

## EAST Search History

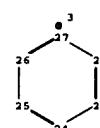
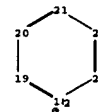
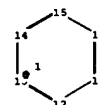
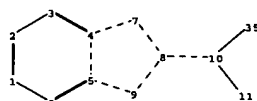
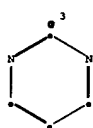
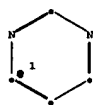
Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	1926	((544/295) or (514/252.14)).CCLS.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	OFF	2006/10/24 19:40

## NPL Search Notes

		Results
4.	TITLE-ABSTR-KEY(blood brain barrier) and TITLE-ABSTR-KEY(jnk and (inhibition or inhibit) and ischemia) [All Sources(- All Sciences -)]	3
3.	TITLE-ABSTR-KEY((expression or activity)) and TITLE-ABSTR-KEY(jnk and (inhibition or inhibit) and ischemia) [All Sources(- All Sciences -)]	88
2.	TITLE-ABSTR-KEY((expression or activity)) and TITLE-ABSTR-KEY(jnk and (inhibition or inhibit)) [All Sources(- All Sciences -)]	3033
1.	TITLE-ABSTR-KEY((expression or activity)) and TITLE-ABSTR-KEY(jnk) [All Sources(- All Sciences -)]	7878

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chain nodes :

10 11 35

ring nodes :

1 2 3 4 5 6 7 8 9 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29

chain bonds :

8-10 10-11 10-35

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9 12-13 12-17 13-14 14-15 15-16 16-17 18-19 18-23  
19-20 20-21 21-22 22-23 24-25 24-29 25-26 26-27 27-28 28-29

exact/norm bonds :

4-5 4-7 5-9 7-8 8-9 8-10 10-35

exact bonds :

10-11

normalized bonds :

1-2 1-6 2-3 3-4 5-6 12-13 12-17 13-14 14-15 15-16 16-17 18-19 18-23 19-20 20-21 21-22  
22-23 24-25 24-29 25-26 26-27 27-28 28-29

isolated ring systems :

containing 1 : 12 : 18 : 24 :

G1:[\*1],[\*2],[\*3]

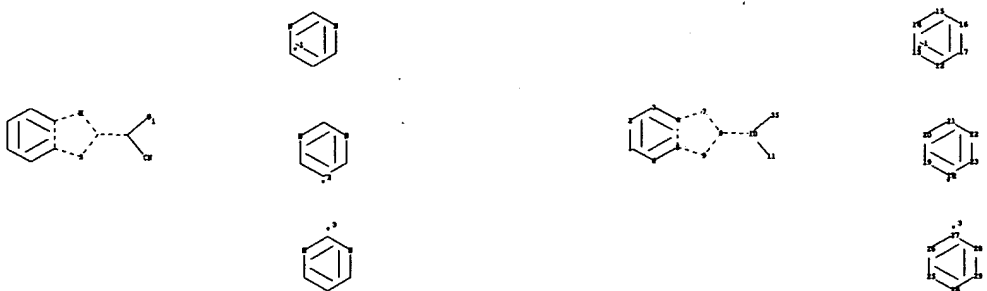
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS11:CLASS12:Atom  
13:Atom

14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom  
24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 35:CLASS

=&gt;

Uploading C:\Program Files\Stnexp\Queries\10168718.str



chain nodes :

10 11 35

ring nodes :

1 2 3 4 5 6 7 8 9 12 13 14 15 16 17 18 19 20 21 22 23 24 25  
26 27 28 29

chain bonds :

8-10 10-11 10-35

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-9 7-8 8-9 12-13 12-17 13-14 14-15 15-16  
16-17 18-19 18-23 19-20 20-21 21-22 22-23 24-25 24-29 25-26 26-27 27-28  
28-29

exact/norm bonds :

4-5 4-7 5-9 7-8 8-9 8-10 10-35

exact bonds :

10-11

normalized bonds :

1-2 1-6 2-3 3-4 5-6 12-13 12-17 13-14 14-15 15-16 16-17 18-19 18-23  
19-20 20-21 21-22 22-23 24-25 24-29 25-26 26-27 27-28 28-29

isolated ring systems :

containing 1 : 12 : 18 : 24 :

G1:[\*1],[\*2],[\*3]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
 11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom  
 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom  
 29:Atom 35:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

SAMPLE SEARCH INITIATED 14:19:34 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 19 TO ITERATE

100.0% PROCESSED 19 ITERATIONS

17 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 119 TO 641

PROJECTED ANSWERS: 93 TO 587

L2 17 SEA SSS SAM L1

=> => s l1 sss ful

FULL SEARCH INITIATED 14:20:49 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 278 TO ITERATE

100.0% PROCESSED 278 ITERATIONS

266 ANSWERS

SEARCH TIME: 00.00.01

L3 266 SEA SSS FUL L1

=> => s l3

L4 16 L3

=> d l4 1-16 bib,ab,hitstr

L4 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2006:769183 CAPLUS  
 DN 145:181019  
 TI Use of inhibitors of jun N-terminal kinases to treat glaucoma  
 IN Fleenor, Debra L.; Pang, Iok-Hou  
 PA Alcon, Inc., USA  
 SO U.S. Pat. Appl. Publ., 14pp., Cont.-in-part of U.S. Ser. No. 259,566.  
 CODEN: USXXCO

DT Patent  
 LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2006172991	A1	20060803	US 2006-394893	20060331
	US 2006094753	A1	20060504	US 2005-259566	20051026
PRAI	US 2004-623755P	P	20041029		
	US 2005-259566	A2	20051026		

AB Compns. and methods for lowering intraocular pressure (IOP) and/or providing neuroprotection are disclosed. The compns. and methods are particularly directed to the use inhibitors of Jun N-terminal kinases (JNK) to lower IOP and/or provide neuroprotection.

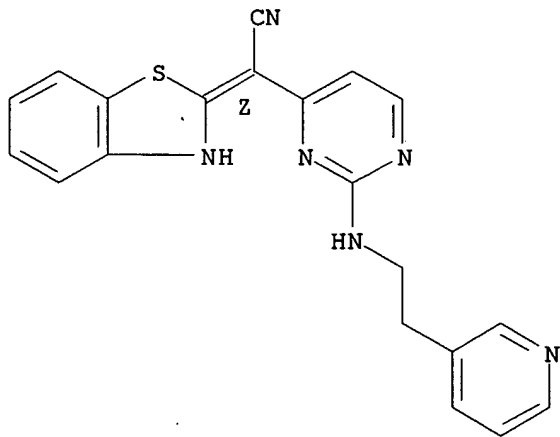
IT 861411-83-8

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (JNK kinase inhibitors for treatment of glaucoma)

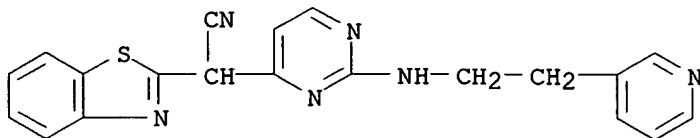
RN 861411-83-8 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(3-pyridinyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

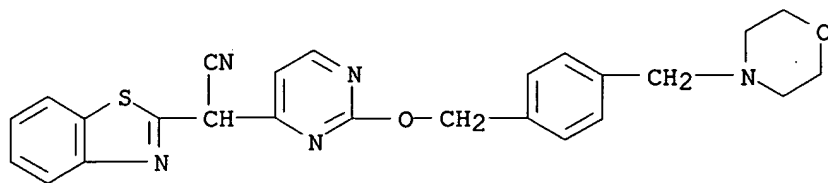


L4 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2006:763978 CAPLUS  
 DN 145:159088  
 TI Designing heterocyclic selective kinase inhibitors: from concept to new drug candidates  
 AU Halazy, Serge  
 CS Serono Pharmaceutical Research Institute, Geneva, Switz.  
 SO ARKIVOC (Gainesville, FL, United States) (2006), (7), 496-508  
 CODEN: AGFUAR  
 URL: [http://www.arkat-usa.org/ARKIVOC/JOURNAL\\_CONTENT/manuscripts/2006/HL-1867GR%20as%20published%20mainmanuscript.pdf](http://www.arkat-usa.org/ARKIVOC/JOURNAL_CONTENT/manuscripts/2006/HL-1867GR%20as%20published%20mainmanuscript.pdf)castype  
 PB Arkat USA Inc.  
 DT Journal; (online computer file)  
 LA English  
 AB Kinases represent one of the most popular and promising target class in drug discovery. Success in finding new therapeutics will depend on the validation of the kinase chosen with respect to the disease of interest, and on the ability of chemists to design and synthesize inhibitors which are selective for this particular kinase. One of the most powerful validation tool for kinases is the Analog-Sensitive Kinase Allele (ASKA) technol., where chemists and biologists have engineered modified kinases and inhibitors by generating functionally active kinase mutants which are specifically inhibited by a chemical modified inhibitor, thus allowing to study specific responses in knock-in animals. The design of selective, ATP competitive kinase inhibitors has been successfully achieved by combining different technologies like computational chemical, structure-based design and combinatorial chemical as illustrated by the discovery of AS602801, a potent and selective JNK inhibitor with therapeutic potential in MS and fibrosis. The exploration of non ATP-competitive inhibitors is also very promising, as illustrated by the case of MEK inhibitors which show strong interest as anti-cancer agents. In the future, the rationale design of selective kinase inhibitors will move to the design of compds. that will induce a selective perturbation of cell regulation, where kinases play a critical role.  
 IT 345987-15-7, AS601245 848344-36-5, AS 602801  
 RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (designing heterocyclic selective kinase inhibitors)  
 RN 345987-15-7 CAPLUS  
 CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(3-pyridinyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 848344-36-5 CAPLUS  
 CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[4-(4-morpholinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

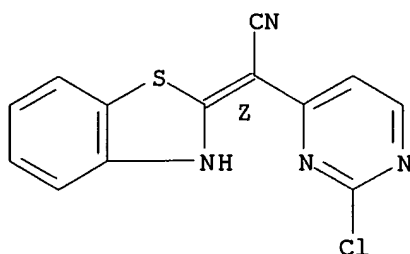




RE: CNT 19      THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2006:506341 CAPLUS  
 DN 145:95781  
 TI Exploration of a Binding Mode of Benzothiazol-2-yl Acetonitrile Pyrimidine  
 Core Based Derivatives as Potent c-Jun N-Terminal Kinase-3 Inhibitors and  
 3D-QSAR Analyses  
 AU Sharma, Pooja; Ghoshal, Nanda  
 CS Drug Design Development and Molecular Modeling Division, Indian Institute  
 of Chemical Biology (CSIR), Kolkata, 700032, India  
 SO Journal of Chemical Information and Modeling (2006), 46(4), 1763-1774  
 CODEN: JCISD8; ISSN: 1549-9596  
 PB American Chemical Society  
 DT Journal  
 LA English  
 AB C-Jun N-terminal kinase (JNK) is a therapeutic target for inhibitors which  
 may provide clin. benefit in the pathogenesis of rheumatoid arthritis (RA)  
 as well as in various apoptosis-related disorders. The benzothiazol-2-yl  
 acetonitrile derivs., recently reported by Pascale et al. (J. Med.  
 Chem.2005, 48, 4596-4607), are the first generation JNK inhibitors of this  
 class. To understand inhibitory mechanisms and elucidate pharmacophoric  
 properties of these derivs. mol. docking and 3D-QSAR studies were  
 performed on a set of 44 compds. Ligand Fit module of Cerius2 (4.9) was  
 employed to locate the binding orientations of all the compds. within the  
 JNK-3 ATP binding site. A good correlation ( $r^2=0.810$ ) between the calculated  
 binding free energies (-PMF score) and the exptl. inhibitory activities  
 suggests that the identified binding conformations of these potential  
 inhibitors are reliable. Based on the binding conformations, robust and  
 highly predictive 3D-QSAR models were developed with conventional  $r^2$  0.886  
 and 0.802, full cross-validation  $r^2$  0.980 and 0.788, and predictive  $r^2$   
 0.965 and 0.968 for MFA and MSA, resp. The interaction mode was  
 demonstrated taking into consideration inhibitor conformation, hydrogen  
 bonding, and electrostatic interaction. The 3D-QSAR model built in this  
 study will provide clear guidelines for a novel inhibitor design based on  
 the benzothiazole derivs. against JNK-3 for the treatment of inflammatory  
 disorders.  
 IT 861411-30-5 861411-33-8 861411-37-2  
 861411-38-3 861411-39-4 861411-40-7  
 861411-41-8 861411-42-9 861411-43-0  
 861411-45-2 861411-46-3 861411-47-4  
 861411-48-5 861411-49-6 861411-51-0  
 861411-52-1 861411-53-2 861411-54-3  
 861411-55-4 861411-56-5 861411-57-6  
 861411-58-7 861411-60-1 861411-61-2  
 861411-62-3 861411-63-4 861411-66-7  
 861411-67-8 861411-73-6 861411-74-7  
 861411-75-8 861411-76-9 861411-77-0  
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 861411-81-6 861411-82-7 861411-83-8  
 861411-84-9 861411-85-0 861411-86-1  
 895538-16-6 895538-17-7  
 RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic  
 use); BIOL (Biological study); USES (Uses)  
 (QSAR and binding mode of benzothiazolyl acetonitrile pyrimidine core  
 based derivs. as potent c-Jun N-terminal kinase-3 inhibitors)  
 RN 861411-30-5 CAPLUS  
 CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-chloro-,  
 ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

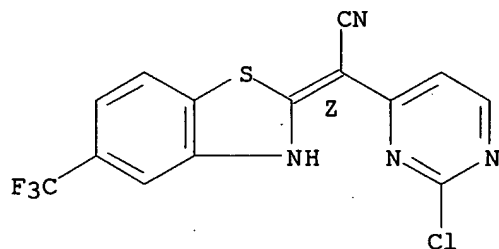
Double bond geometry as shown.



RN 861411-33-8 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-chloro- $\alpha$ -[5-(trifluoromethyl)-2(3H)-benzothiazolylidene]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

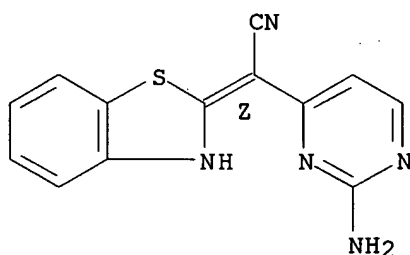
Double bond geometry as shown.



RN 861411-37-2 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-amino- $\alpha$ -2(3H)-benzothiazolylidene-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

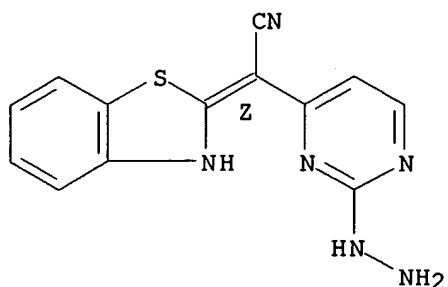
Double bond geometry as shown.



RN 861411-38-3 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-hydrazino-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

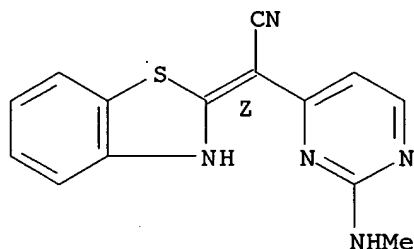
Double bond geometry as shown.



RN 861411-39-4 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-(methylamino)-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

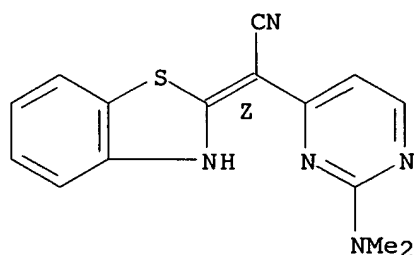
Double bond geometry as shown.



RN 861411-40-7 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-(dimethylamino)-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

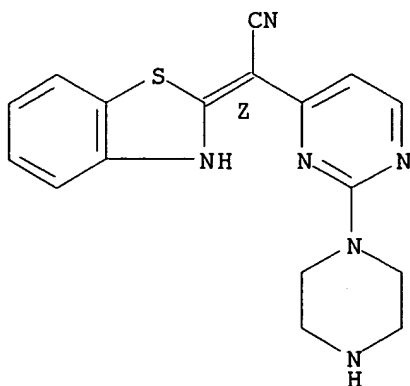
Double bond geometry as shown.



RN 861411-41-8 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-(1-piperazinyl)-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

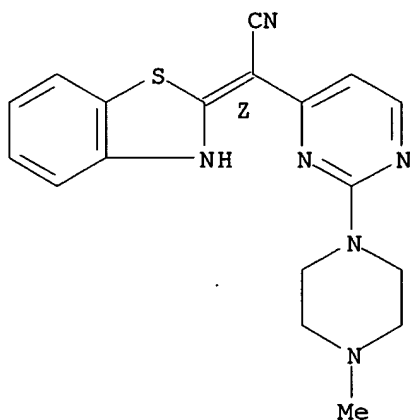
Double bond geometry as shown.



RN 861411-42-9 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-(4-methyl-1-piperazinyl)-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

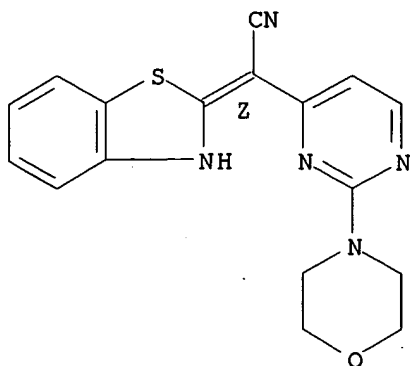
Double bond geometry as shown.



RN 861411-43-0 CAPLUS

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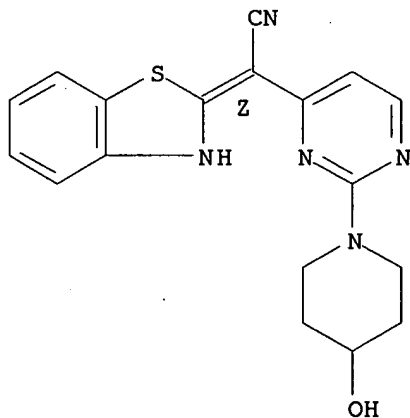
Double bond geometry as shown.



RN 861411-45-2 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-(4-hydroxy-1-piperidinyl)-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

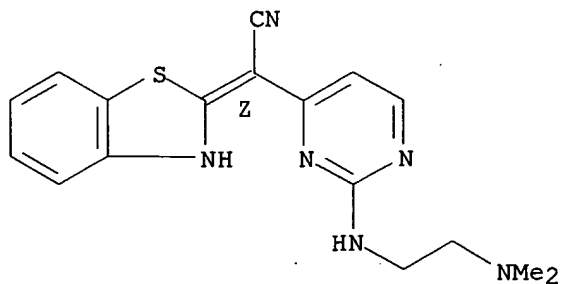
Double bond geometry as shown.



RN 861411-46-3 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(dimethylamino)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

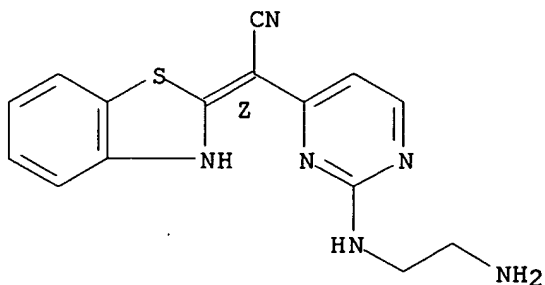
Double bond geometry as shown.



RN 861411-47-4 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-[(2-aminoethyl)amino]- $\alpha$ -2(3H)-benzothiazolylidene-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

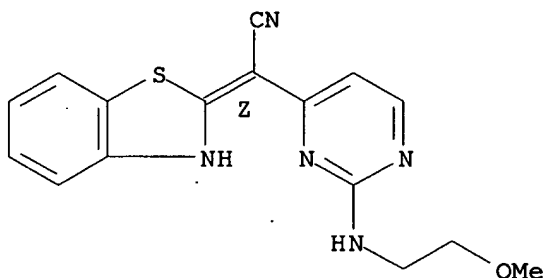
Double bond geometry as shown.



RN 861411-48-5 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[(2-methoxyethyl)amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

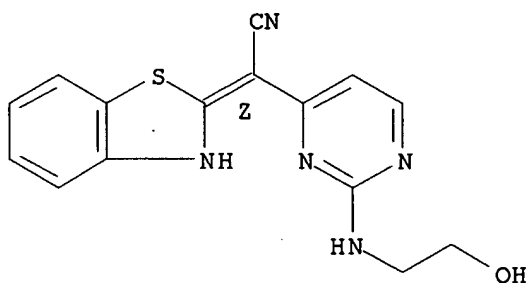
Double bond geometry as shown.



RN 861411-49-6 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[(2-hydroxyethyl)amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

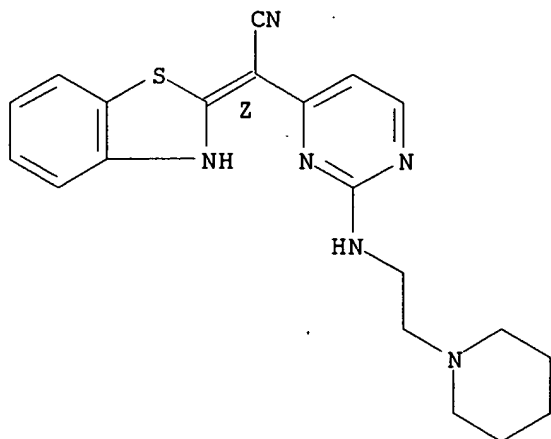
Double bond geometry as shown.



RN 861411-51-0 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(1-piperidinyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

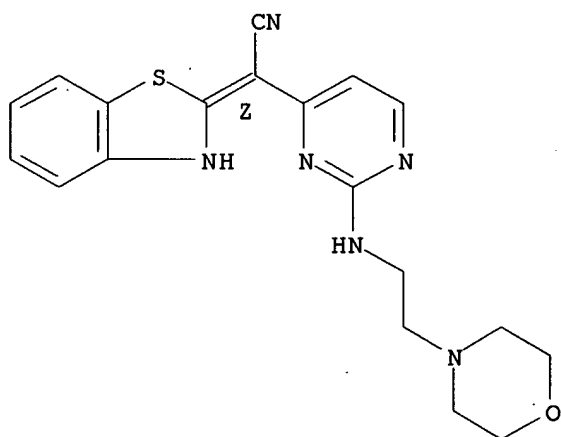
Double bond geometry as shown.



RN 861411-52-1 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(4-morpholinyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

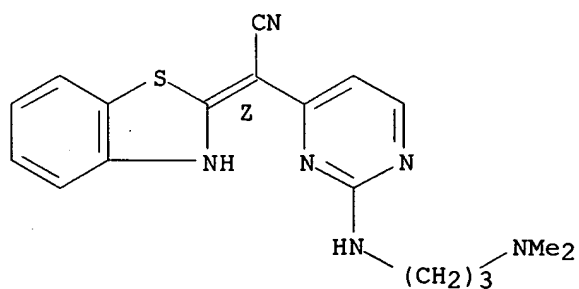
Double bond geometry as shown.



RN 861411-53-2 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[3-(dimethylamino)propyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

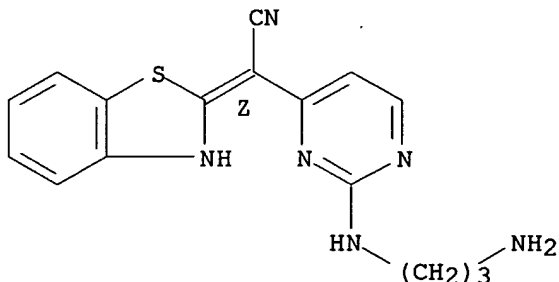




RN 861411-54-3 CAPLUS

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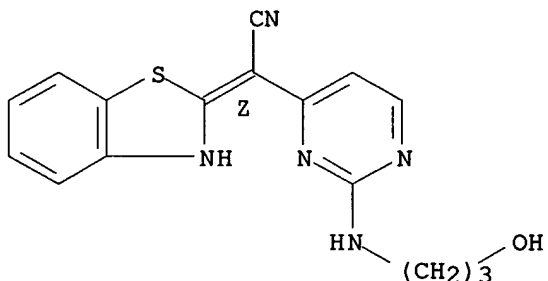
Double bond geometry as shown.



RN 861411-55-4 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[(3-hydroxypropyl)amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

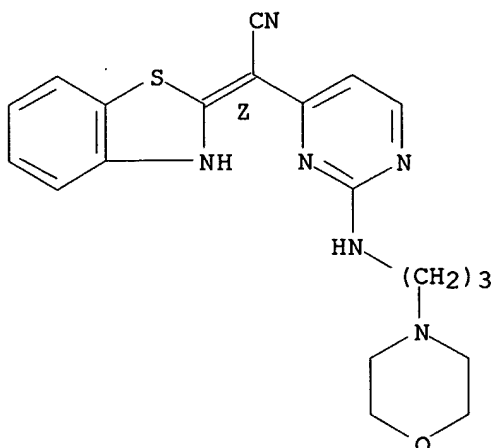
Double bond geometry as shown.



RN 861411-56-5 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[3-(4-morpholinyl)propyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

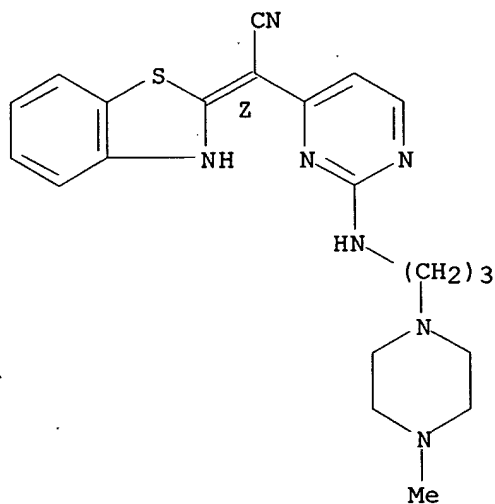
Double bond geometry as shown.



RN 861411-57-6 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[3-(4-methyl-1-piperazinyl)propyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

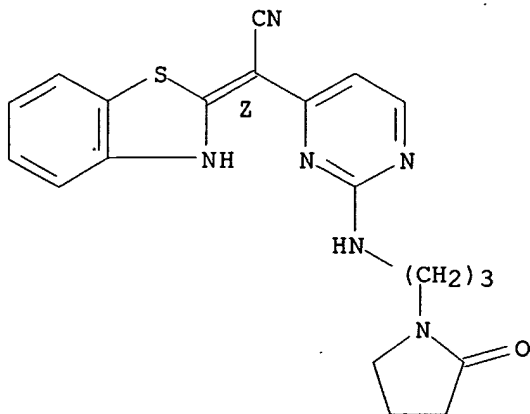
Double bond geometry as shown.



RN 861411-58-7 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[3-(2-oxo-1-pyrrolidinyl)propyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

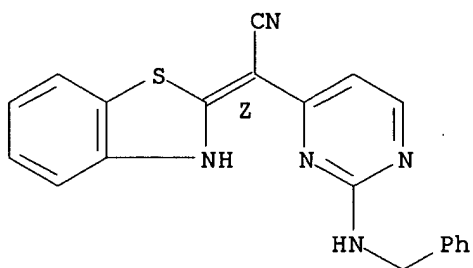
Double bond geometry as shown.



RN 861411-60-1 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[(phenylmethyl)amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

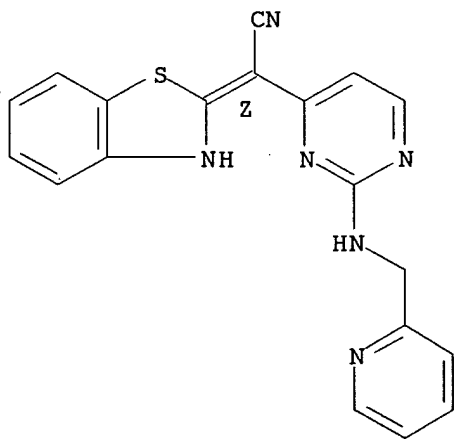
Double bond geometry as shown.



RN 861411-61-2 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[(2-pyridinylmethyl)amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

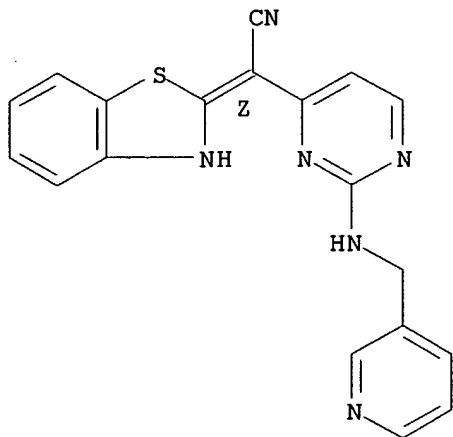
Double bond geometry as shown.



RN 861411-62-3 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[(3-pyridinylmethyl)amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

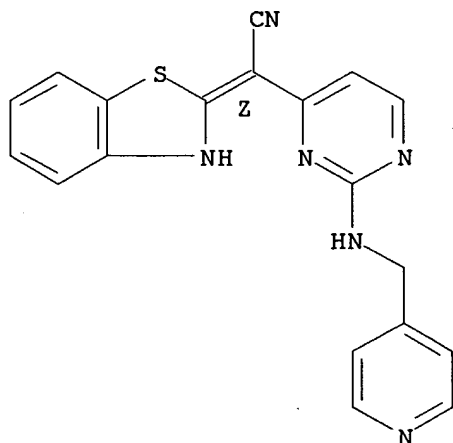
Double bond geometry as shown.



RN 861411-63-4 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[(4-pyridinylmethyl)amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

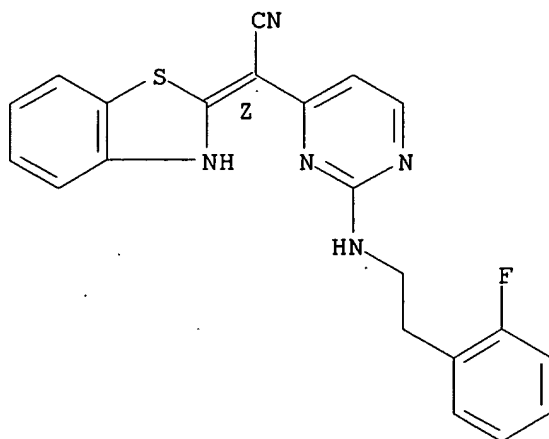
Double bond geometry as shown.



RN 861411-66-7 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(2-fluorophenyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

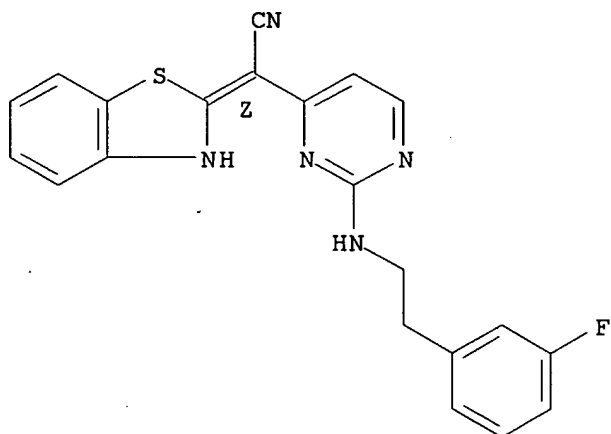
Double bond geometry as shown.



RN 861411-67-8 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(3-fluorophenyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

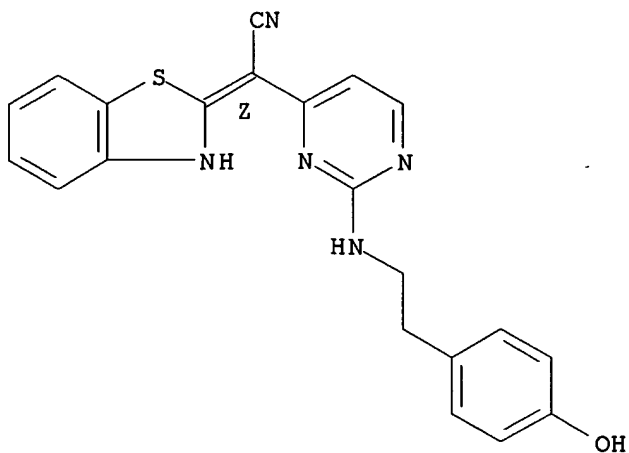
Double bond geometry as shown.



RN 861411-73-6 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(4-hydroxyphenyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

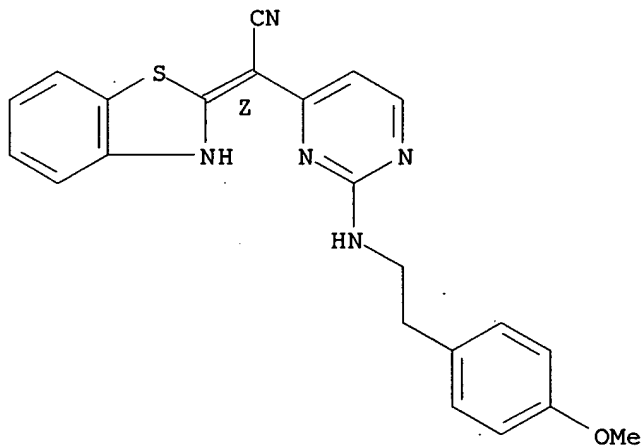
Double bond geometry as shown.



RN 861411-74-7 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(4-methoxyphenyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

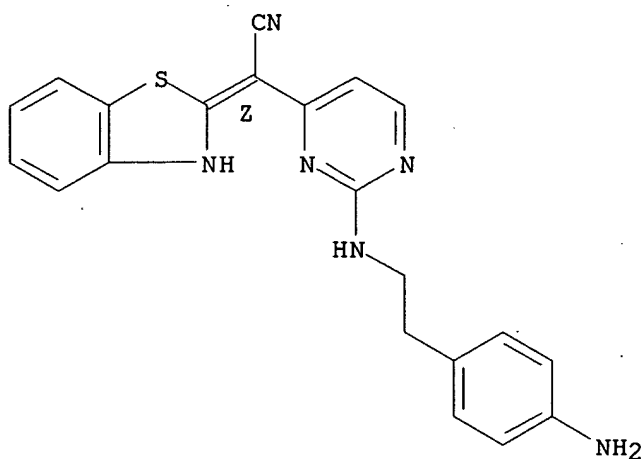
Double bond geometry as shown.



RN 861411-75-8 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-[[2-(4-aminophenyl)ethyl]amino]- $\alpha$ -2(3H)-benzothiazolylidene-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

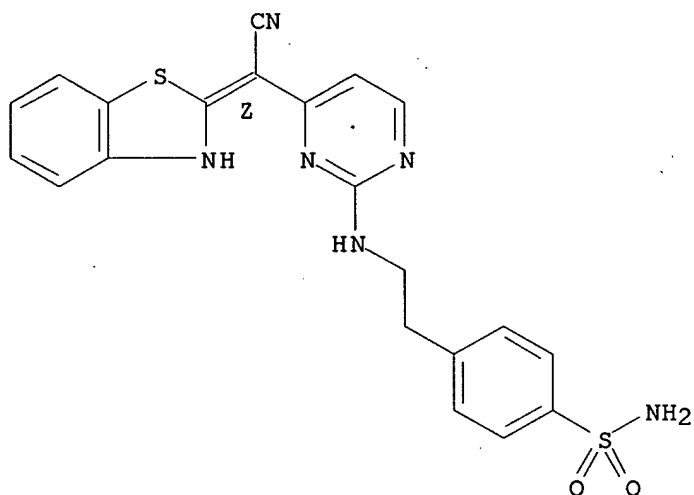
Double bond geometry as shown.



RN 861411-76-9 CAPLUS

CN Benzenesulfonamide, 4-[2-[[4-[(Z)-2(3H)-benzothiazolylidenecyanomethyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

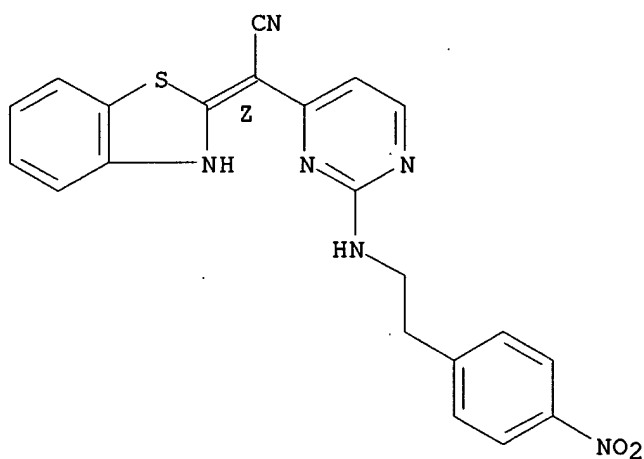
Double bond geometry as shown.



RN 861411-77-0 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(4-nitrophenyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

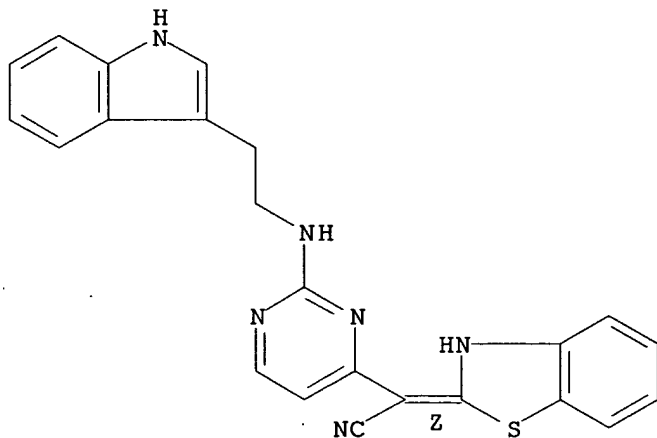
Double bond geometry as shown.



RN 861411-78-1 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(1H-indol-3-yl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

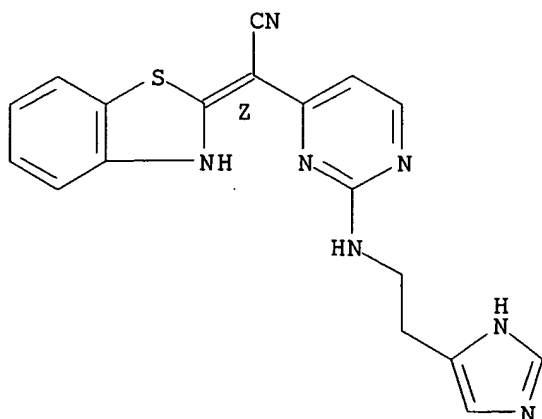


RN 861411-79-2 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(1H-imidazol-4-yl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

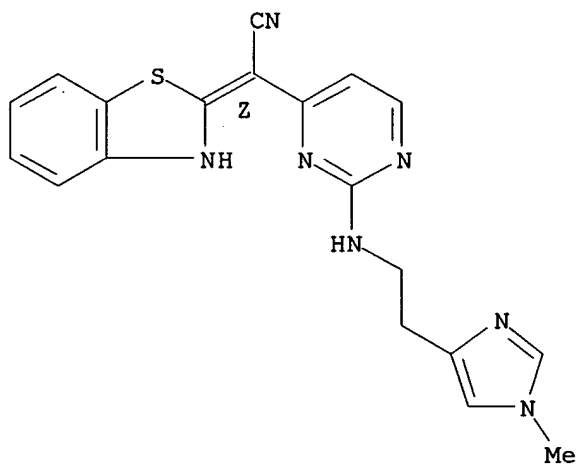




RN 861411-80-5 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(1-methyl-1H-imidazol-4-yl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

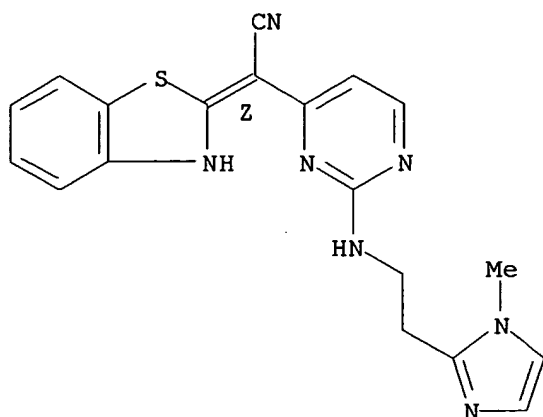
Double bond geometry as shown.



RN 861411-81-6 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[2-(1-methyl-1H-imidazol-2-yl)ethyl]amino]-, (αZ)- (9CI) (CA INDEX NAME)

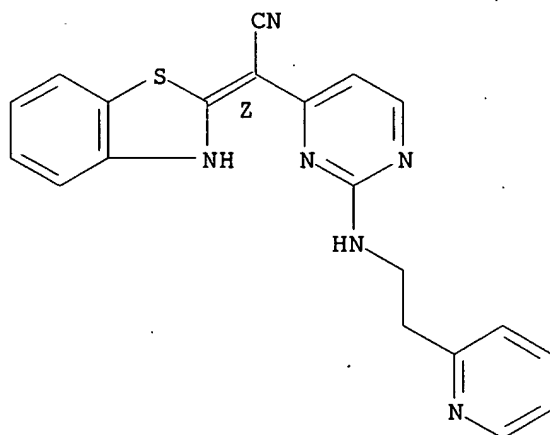
Double bond geometry as shown.



RN 861411-82-7 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(2-pyridinyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

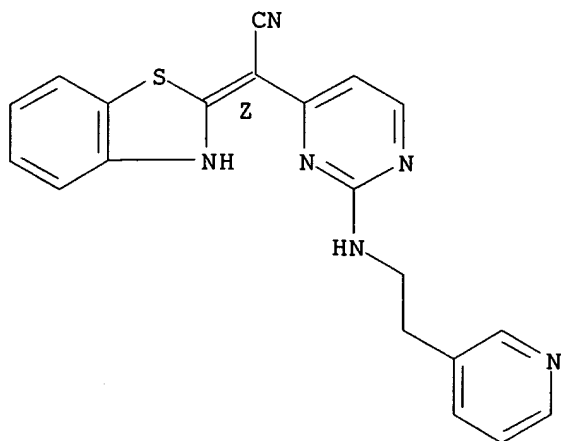
Double bond geometry as shown.



RN 861411-83-8 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(3-pyridinyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

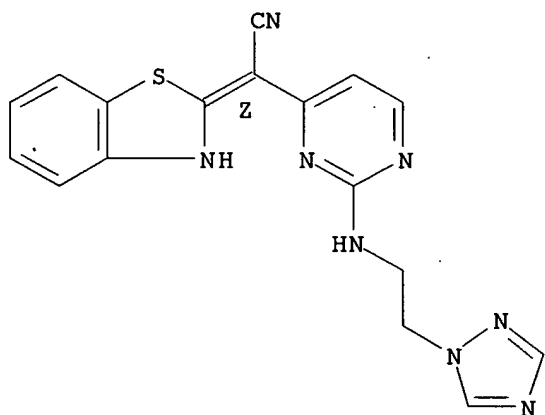
Double bond geometry as shown.



RN 861411-84-9 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(1H-1,2,4-triazol-1-yl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

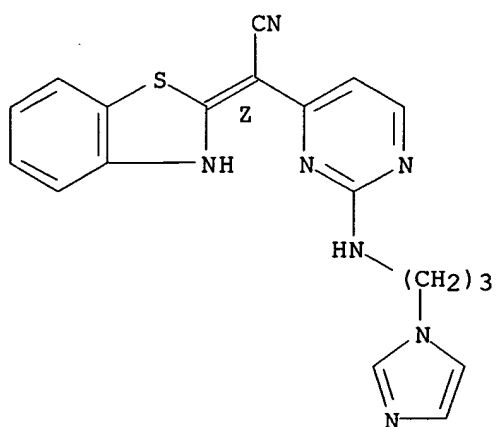
Double bond geometry as shown.



RN 861411-85-0 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[3-(1H-imidazol-1-yl)propyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

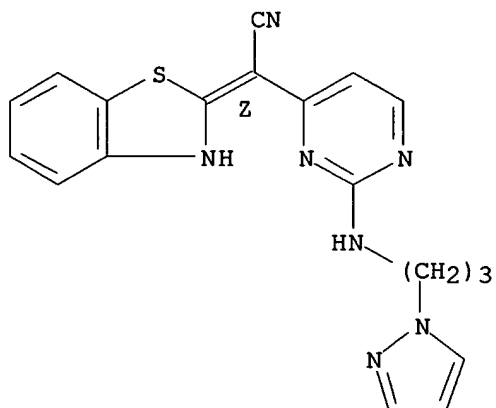
Double bond geometry as shown.



RN 861411-86-1 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[3-(1H-pyrazol-1-yl)propyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

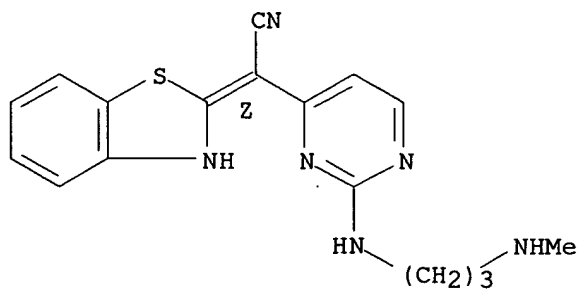
Double bond geometry as shown.



RN 895538-16-6 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[3-(methylamino)propyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

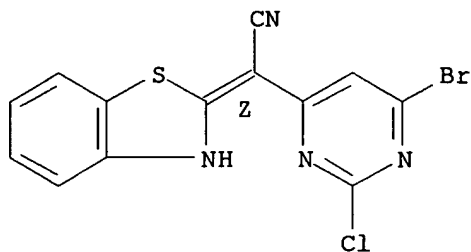
Double bond geometry as shown.



RN 895538-17-7 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-6-bromo-2-chloro-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RE.CNT 75 THERE ARE 75 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2006:496089 CAPLUS

DN 145:8158

TI Preparation of benzothiazoles, their macrogol glyceride pharmaceutical formulations, and their therapeutic use

IN Esposito, Pierandrea; Chicco, Daniela; Donati, Luca; Leonardi, Andrea; Bertero, Stefania; Gotteland, Jean-Pierre; Gaillard, Pascale; Jeanclaude-Etter, Isabelle; Grandolini, Simone; Maio, Mario

PA Ares Trading S.A., Switz.

SO PCT Int. Appl., 95 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2006053882	A2	20060526	WO 2005-EP56020	20051116
	WO 2006053882	A3	20060908		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRAI EP 2004-105843 A 20041117

US 2004-628998P P 20041118

OS MARPAT 145:8158

AB The invention is related to macrogol glyceride pharmaceutical formulations containing benzothiazoles I [G = pyrimidinyl; L = alkoxy, NH<sub>2</sub>, 3-8 membered heterocycloalkyl containing ≥ 1 heteroatom selected from N, O, and S; R<sub>1</sub> = H, NH<sub>2</sub>, CN, alk(en/yn)yl, etc.], as well as their tautomers, geometrical isomers, enantiomers, diastereomers, racemates, as well as their pharmaceutically acceptable salts. In particular, the invention is related to benzothiazole stearyl macrogol pharmaceutical formulations, method of preparation and use thereof. The invention is also related to the preparation of benzothiazoles I. Thus, benzothiazole II was prepared by reacting

(1,3-benzothiazol-2-yl)acetonitrile with 2,4-dichloropyrimidine, followed by O-alkylation of 3-(2-hydroxyethyl)pyridine with the chloride intermediate. A stearyl macrogol pharmaceutical formulation containing 20% weight/weight III dimesylate and 80% weight/weight Gelucire 50/13 (IV) was

prepared I

are useful for treating fibrosis, asthma, endometriosis, etc (no data).

IT 888070-08-4P, (1,3-Benzothiazol-2-yl)[2-[2-(pyridin-3-yl)ethoxy]pyrimidin-4-yl]acetonitrile 888070-09-5P, (1,3-Benzothiazol-2-yl)[2-[(quinolin-6-yl)oxy]pyrimidin-4-yl]acetonitrile 888070-10-8P 888070-11-9P, (1,3-Benzothiazol-2-yl)[2-[[3-[(4-methylpiperazin-1-yl)methyl]benzyl]oxy]pyrimidin-4-yl]acetonitrile 888070-12-0P 888070-13-1P, (1,3-Benzothiazol-2-yl)[2-(hexyloxy)pyrimidin-4-yl]acetonitrile 888070-14-2P, (1,3-Benzothiazol-2-yl)[2-[[3-[(morpholin-4-yl)methyl]benzyl]oxy]pyrimidin-4-yl]acetonitrile 888070-15-3P, (1,3-Benzothiazol-2-yl)[2-[[3-

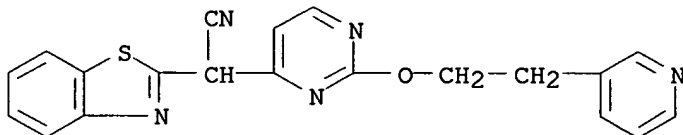
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 888070-16-4P, (1,3-Benzothiazol-2-yl)[2-[[3-[(piperidin-1-yl)methyl]benzyl]oxy]pyrimidin-4-yl]acetonitrile 888070-17-5P,  
 (1,3-Benzothiazol-2-yl)[2-[[4-[(2,6-dimethylmorpholin-4-yl)methyl]benzyl]oxy]pyrimidin-4-yl]acetonitrile 888070-18-6P  
 888070-19-7P 888070-20-0P, (1,3-Benzothiazol-2-yl)[2-[[4-[(benzylamino)methyl]benzyl]oxy]pyrimidin-4-yl]acetonitrile  
 888070-21-1P, (1,3-Benzothiazol-2-yl)[2-[[2-(morpholin-4-yl)pyridin-4-yl]methoxy]pyrimidin-4-yl]acetonitrile 888070-22-2P  
 , (1,3-Benzothiazol-2-yl)[2-[[2-(piperidin-1-yl)pyridin-4-yl]methoxy]pyrimidin-4-yl]acetonitrile 888070-23-3P,  
 (1,3-Benzothiazol-2-yl)[2-[[2-(morpholin-4-yl)ethoxy]pyrimidin-4-yl]acetonitrile 888070-24-4P 888070-25-5P,  
 (1,3-Benzothiazol-2-yl)[2-[[2-(dimethylamino)ethoxy]pyrimidin-4-yl]acetonitrile 888070-26-6P 888070-27-7P,  
 (1,3-Benzothiazol-2-yl)[2-[[3-(dimethylamino)propoxy]pyrimidin-4-yl]acetonitrile 888070-28-8P, (1,3-Benzothiazol-2-yl)[2-[[2-(4-methylpiperazin-1-yl)ethoxy]pyrimidin-4-yl]acetonitrile  
 888070-29-9P, (1,3-Benzothiazol-2-yl)[2-[[2-[[2-(dimethylamino)ethoxy]ethoxy]pyrimidin-4-yl]acetonitrile  
 888070-30-2P 888070-31-3P 888070-32-4P  
 888070-33-5P 888070-34-6P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzothiazoles, their macrogol glyceride pharmaceutical formulations, and their therapeutic use)

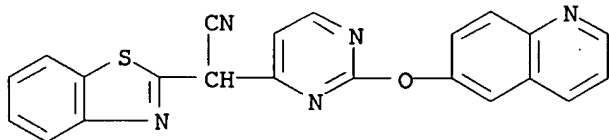
RN 888070-08-4 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(3-pyridinyl)ethoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



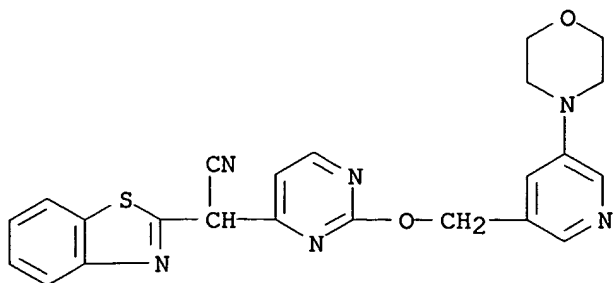
RN 888070-09-5 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(6-quinolinyl)oxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



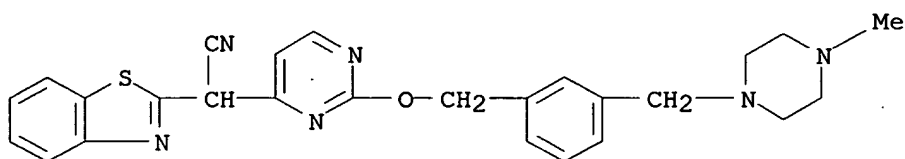
RN 888070-10-8 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[5-(4-morpholinyl)-3-pyridinyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



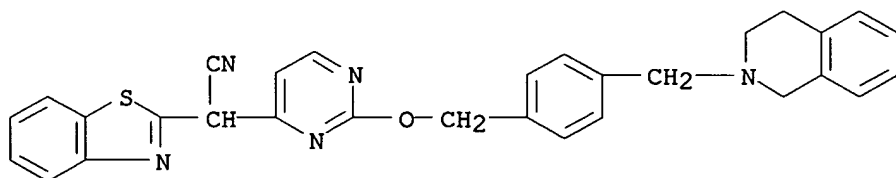
RN 888070-11-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-[(4-methyl-1-piperazinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



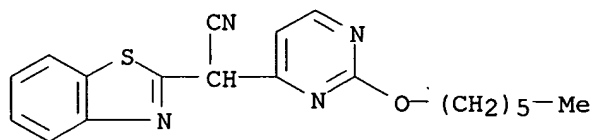
RN 888070-12-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-[(3,4-dihydro-2(1H)-isoquinolinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 888070-13-1 CAPLUS

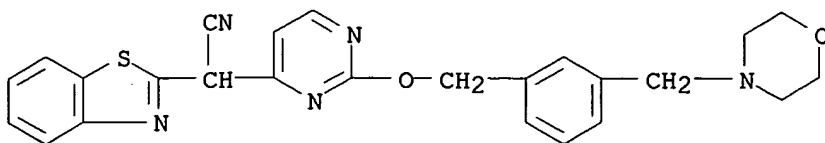
CN 2-Benzothiazoleacetonitrile, α-[2-(hexyloxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 888070-14-2 CAPLUS

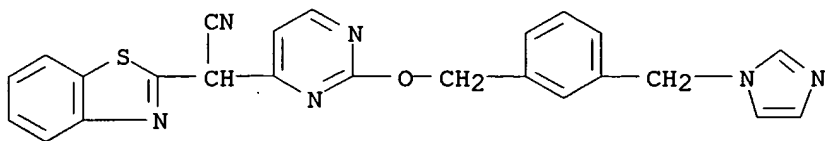
CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(4-morpholinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)





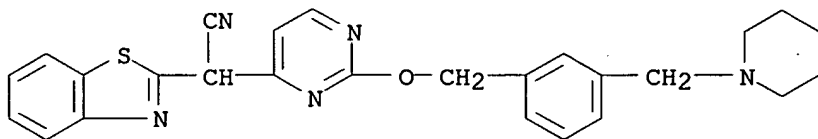
RN 888070-15-3 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[3-(1H-imidazol-1-ylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



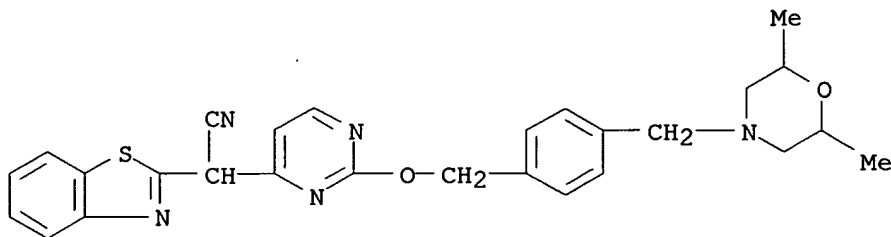
RN 888070-16-4 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[3-(1-piperidinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



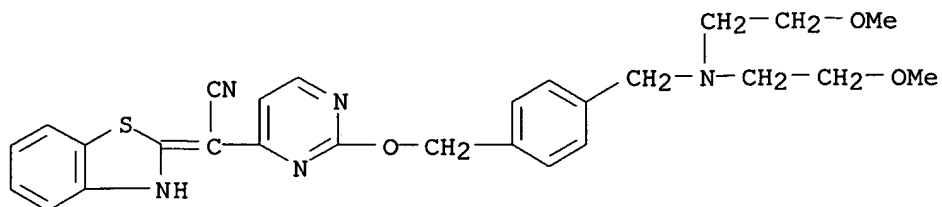
RN 888070-17-5 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[4-[(2,6-dimethyl-4-morpholinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



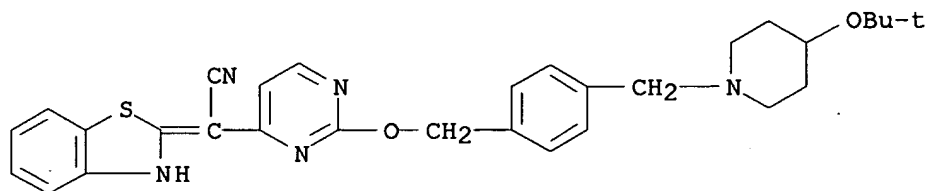
RN 888070-18-6 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[4-[[bis(2-methoxyethyl)amino]methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)



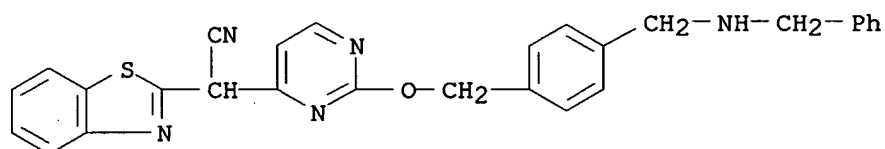
RN 888070-19-7 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolydene-2-[[4-[[4-(1,1-dimethylethoxy)-1-piperidinyl]methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)



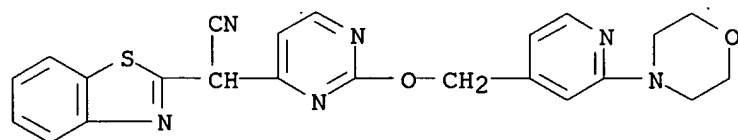
RN 888070-20-0 CAPLUS

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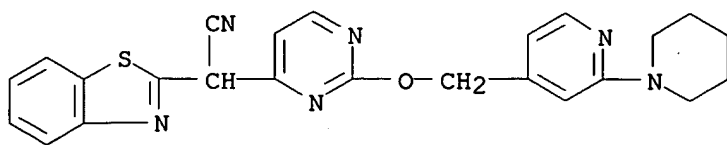
RN 888070-21-1 CAPLUS

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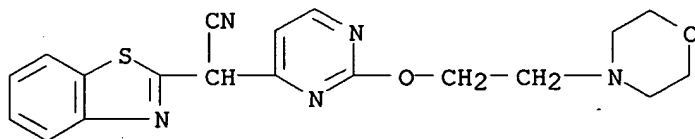
RN 888070-22-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(1-piperidinyl)-4-pyridinyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



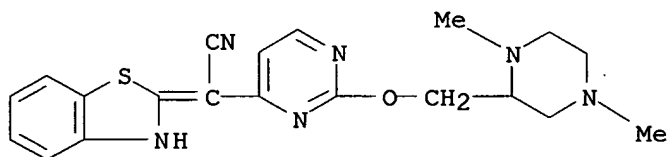
RN 888070-23-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[2-(4-morpholinyl)ethoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



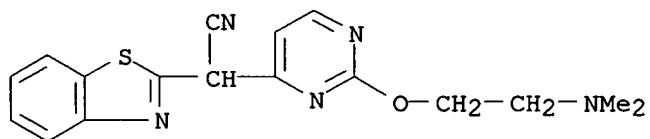
RN 888070-24-4 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[(1,4-dimethyl-2-piperazinyl)methoxy]- (9CI) (CA INDEX NAME)



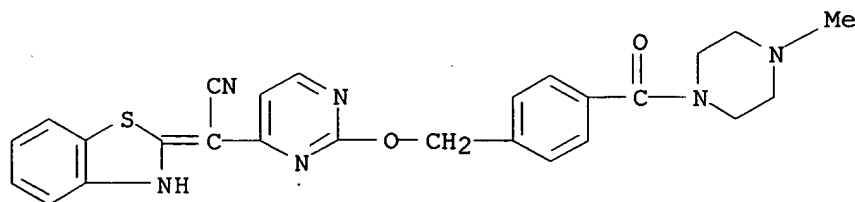
RN 888070-25-5 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[2-(dimethylamino)ethoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

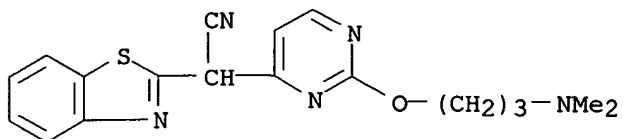


RN 888070-26-6 CAPLUS

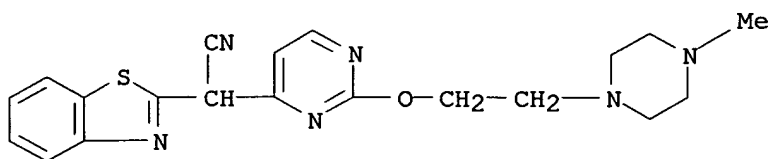
CN Piperazine, 1-[4-[[[4-(2(3H)-benzothiazolyldenecyanomethyl)-2-pyrimidinyl]oxy)methyl]benzoyl]-4-methyl- (9CI) (CA INDEX NAME)



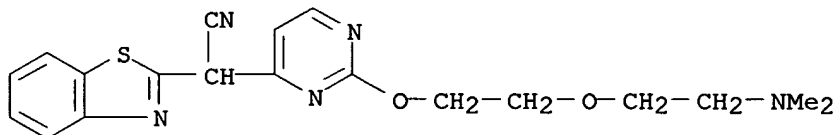
RN 888070-27-7 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[3-(dimethylamino)propoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 888070-28-8 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[2-(4-methyl-1-piperazinyl)ethoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 888070-29-9 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[2-[2-(dimethylamino)ethoxy]ethoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

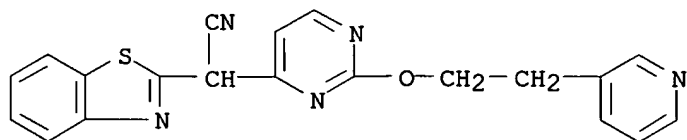
RN 888070-30-2 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[2-(3-pyridinyl)ethoxy]-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

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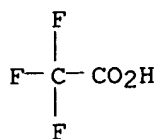
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CM 2

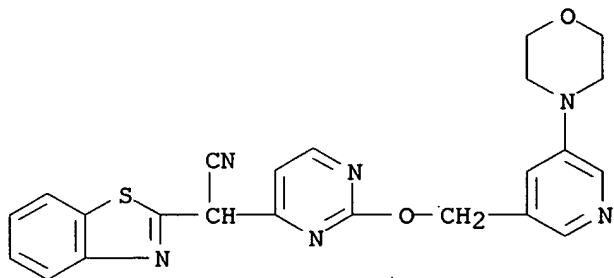
CRN 76-05-1  
CMF C2 H F3 O2



RN 888070-31-3 CAPLUS  
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[5-(4-morpholinyl)-3-pyridinyl]methoxy]-4-pyrimidinyl]-, methanesulfonate (9CI) (CA INDEX NAME)

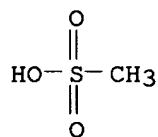
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CM 2

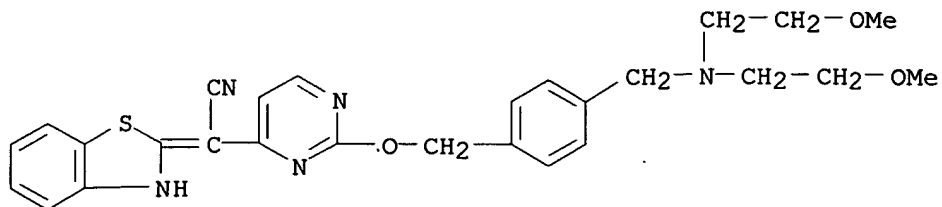
CRN 75-75-2  
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RN 888070-32-4 CAPLUS  
CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[4-[[bis(2-methoxyethyl)amino]methyl]phenyl]methoxy]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

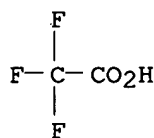
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CM 2

CRN 76-05-1

CMF C2 H F3 O2



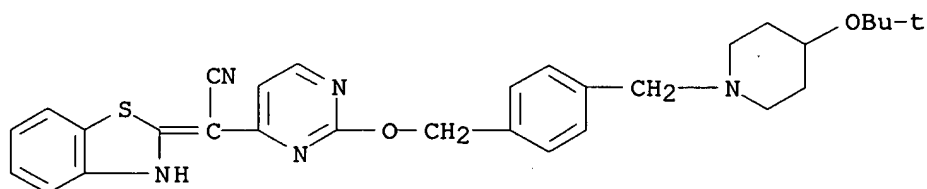
RN 888070-33-5 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[4-[[4-(1,1-dimethylethoxy)-1-piperidinyl]methyl]phenyl]methoxy]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 888070-19-7

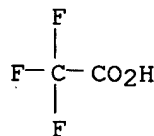
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CM 2

CRN 76-05-1

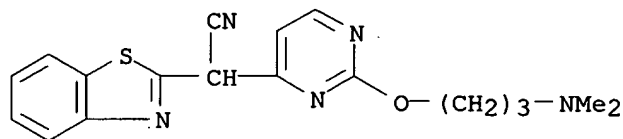
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RN 888070-34-6 CAPLUS  
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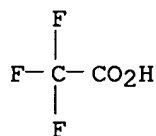
CM 1

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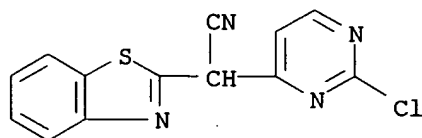


CM 2

CRN 76-05-1  
 CMF C2 H F3 O2



IT 345986-38-1P, (1,3-Benzothiazol-2-yl)(2-chloro-4-pyrimidinyl)acetonitrile  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (intermediate; preparation of benzothiazoles, their macrogol glyceride pharmaceutical formulations, and their therapeutic use)  
 RN 345986-38-1 CAPLUS  
 CN 2-Benzothiazoleacetonitrile,  $\alpha$ -(2-chloro-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

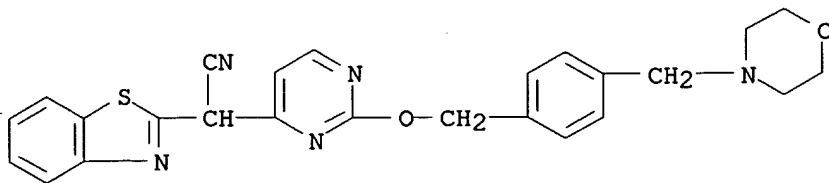


IT 888069-99-6P  
 RL: PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of benzothiazoles, their macrogol glyceride pharmaceutical formulations, and their therapeutic use)  
 RN 888069-99-6 CAPLUS  
 CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[4-(4-morpholinylmethyl)phenyl]methoxy]-4-pyrimidinyl]-, dimethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 848344-36-5

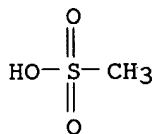
CMF C25 H23 N5 O2 S



CM 2

CRN 75-75-2

CMF C H4 O3 S

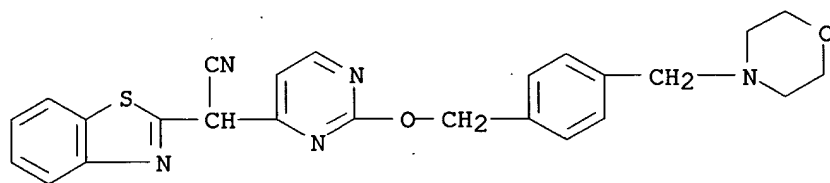


IT 848344-36-5, (1,3-Benzothiazol-2-yl)[2-[[4-[(morpholin-4-yl)methyl]benzyl]oxy]pyrimidin-4-yl]acetonitrile

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(preparation of benzothiazoles, their macrogol glyceride pharmaceutical formulations, and their therapeutic use)

RN 848344-36-5 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[4-(4-morpholinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)





L4 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2005:1123763 CAPLUS  
 DN 143:393032  
 TI Pharmaceutical composition comprising a JNK inhibitor and cyclosporin  
 IN Rommel, Christian; Vitte, Pierre-Alain  
 PA Applied Research Systems Ars Holding N. V., Neth. Antilles  
 SO PCT Int. Appl., 102 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005097116	A1	20051020	WO 2005-EP51572	20050408
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRAI EP 2004-101468 A 20040408

OS MARPAT 143:393032

AB The present invention is related to a composition comprising a c-Jun N-Terminal kinase (JNK) inhibitor and a cyclosporin, in particular for the treatment of neuronal disorders, autoimmune diseases, cancer and cardiovascular diseases. Neuroprotective effects of a JNK inhibitor combined with cyclosporin is shown in a model of global ischemia in gerbils. A JNK inhibitor, e.g. benzothiazole compound was admixed as a dry powder together with a cyclosporin and with a starch diluent in an approx. 1:1 weight ratio. The mixture is filled into 250 mg capsules (125 mg of active benzothiazole compound and 15, 25, or 50 mg of cyclosporin per capsule).

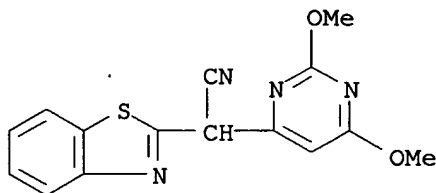
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RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL  
 (Biological study); USES (Uses)  
 (pharmaceutical composition comprising JNK inhibitor and cyclosporin)

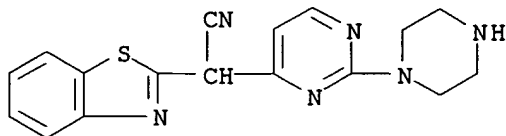
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 (CA INDEX NAME)



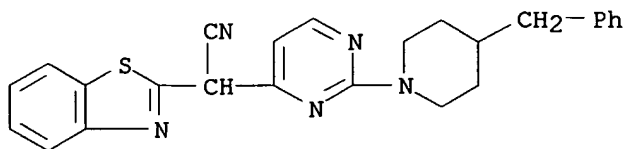
RN 345986-66-5 CAPLUS

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 (9CI) (CA INDEX NAME)



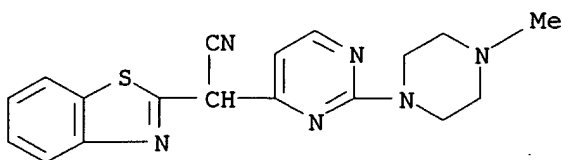
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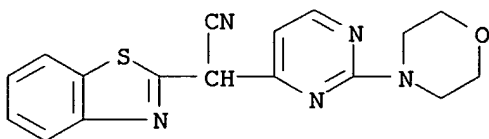
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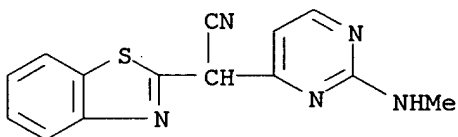
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(9CI) (CA INDEX NAME)



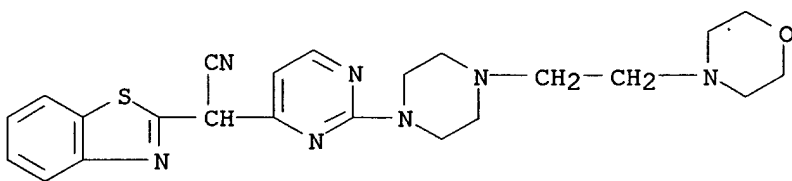
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(9CI) (CA INDEX NAME)



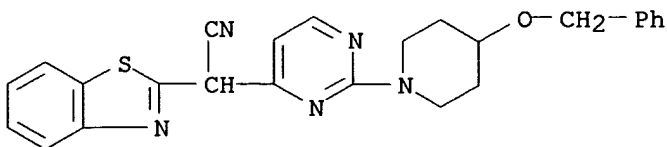
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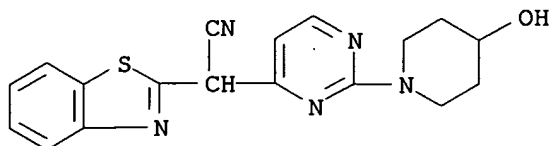


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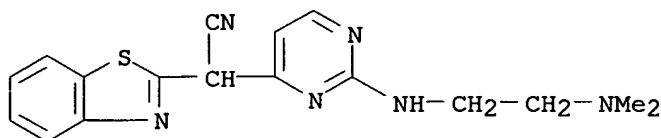
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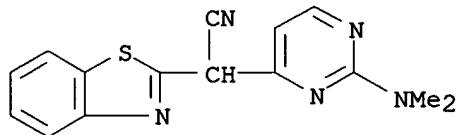
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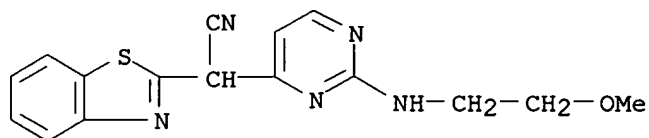
RN 345986-91-6 CAPLUS

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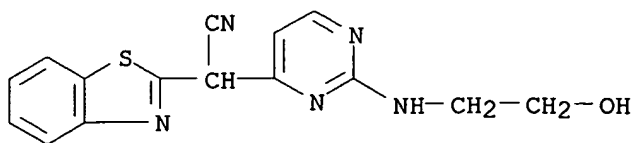
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RN 345986-96-1 CAPLUS

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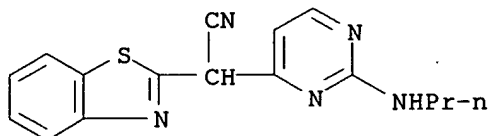
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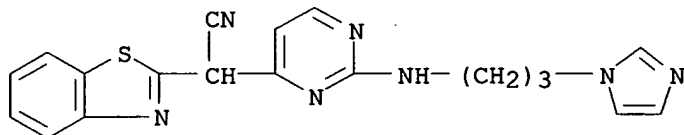
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CN 2-Benzothiazoleacetonitrile, α-[2-(propylamino)-4-pyrimidinyl]-  
(9CI) (CA INDEX NAME)



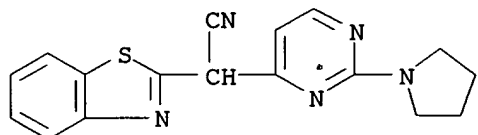
RN 345987-00-0 CAPLUS

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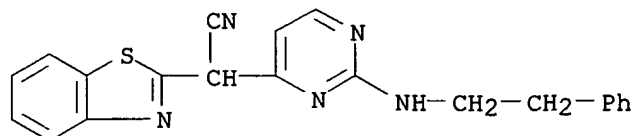
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(9CI) (CA INDEX NAME)



RN 345987-03-3 CAPLUS

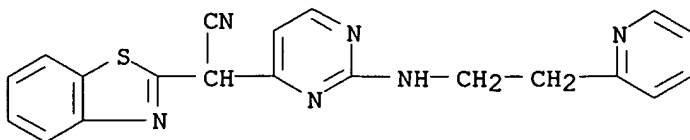
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RN 345987-04-4 CAPLUS

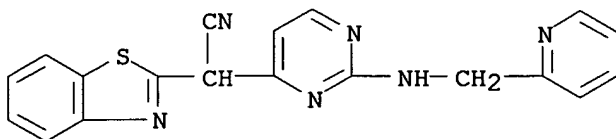
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pyrimidinyl]- (9CI) (CA INDEX NAME)



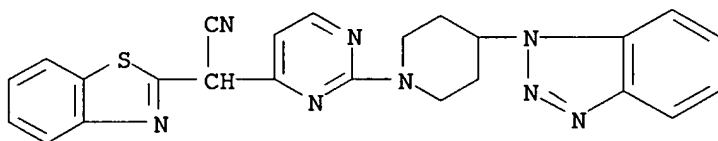
RN 345987-06-6 CAPLUS

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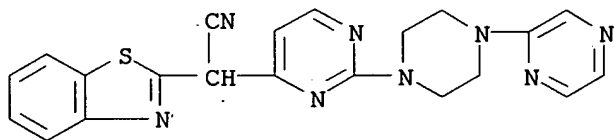
RN 345987-09-9 CAPLUS

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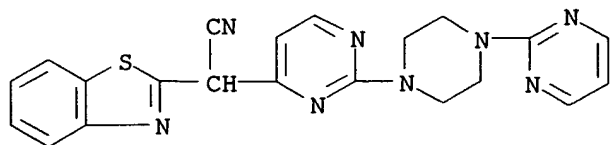
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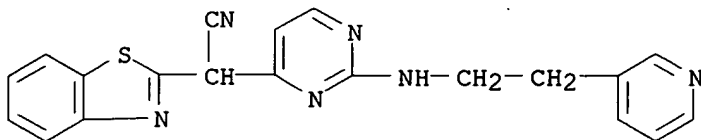


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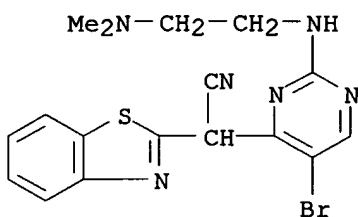
CN 2-Benzothiazoleacetonitrile, α-[2-[4-(2-pyrimidinyl)-1-piperazinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



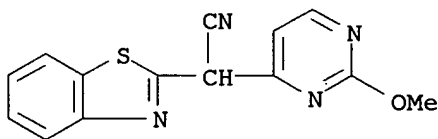
RN 345987-15-7 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(3-pyridinyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

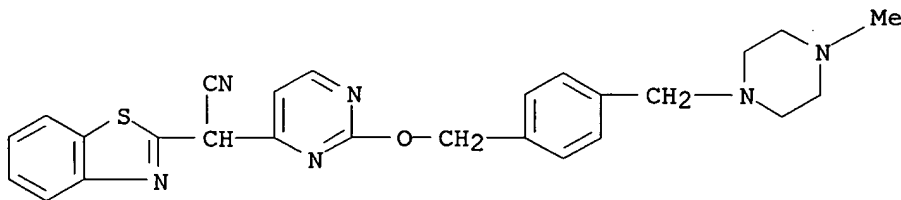
RN 345987-17-9 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[5-bromo-2-[[2-(dimethylamino)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345987-19-1 CAPLUS

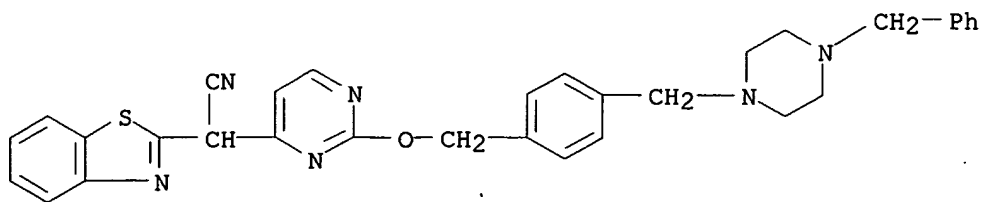
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -(2-methoxy-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

RN 622381-38-8 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[4-[[4-methyl-1-piperazinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

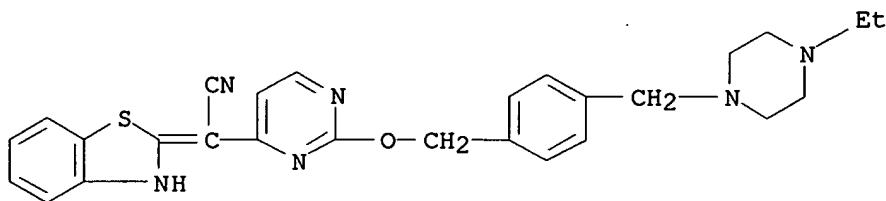
RN 622381-40-2 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[4-[[4-(phenylmethyl)-1-piperazinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 622381-42-4 CAPLUS

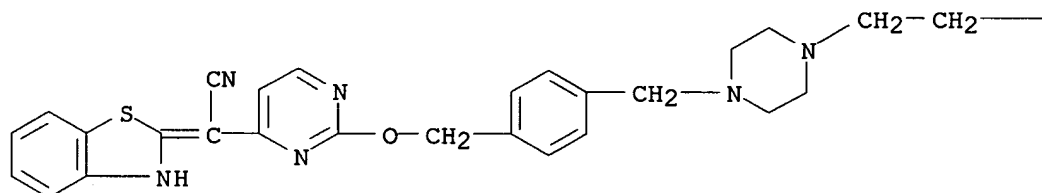
CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[4-[(4-ethyl-1-piperazinyl)methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)



RN 622381-43-5 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[4-[(4-methoxyethyl-1-piperazinyl)methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)

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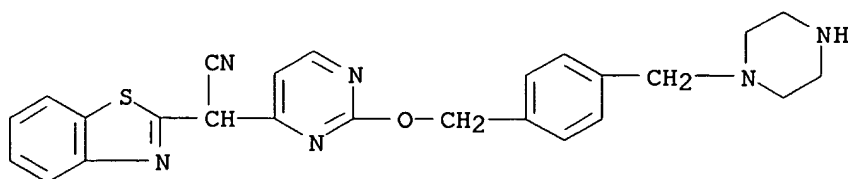


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RN 622381-45-7 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[4-(1-piperazinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

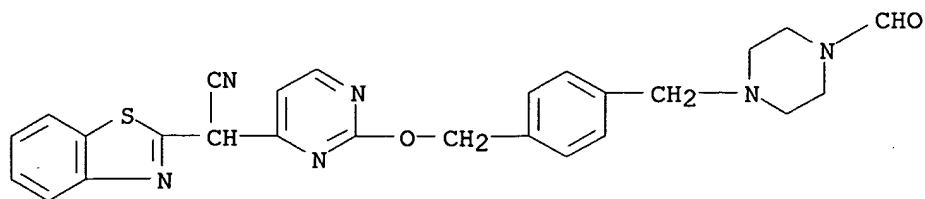


RN 622381-47-9 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[4-(4-formyl-1-

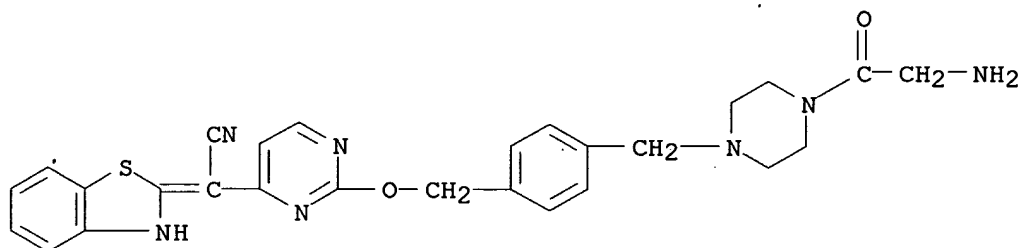


piperazinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



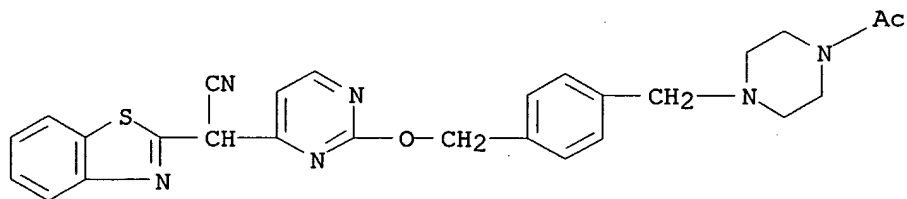
RN 622381-49-1 CAPLUS

CN Piperazine, 1-(aminoacetyl)-4-[[4-[[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy)methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



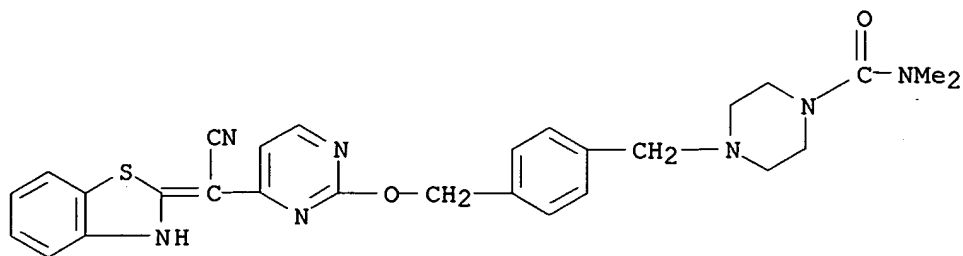
RN 622381-51-5 CAPLUS

CN Piperazine, 1-acetyl-4-[[4-[[[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]oxy)methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



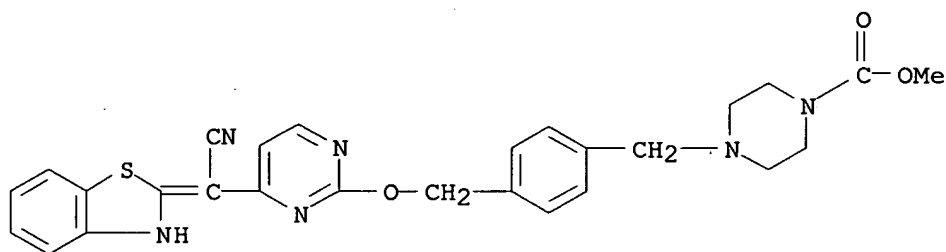
RN 622381-53-7 CAPLUS

CN 1-Piperazinecarboxamide, 4-[[4-[[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy)methyl]phenyl]methyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 622381-55-9 CAPLUS

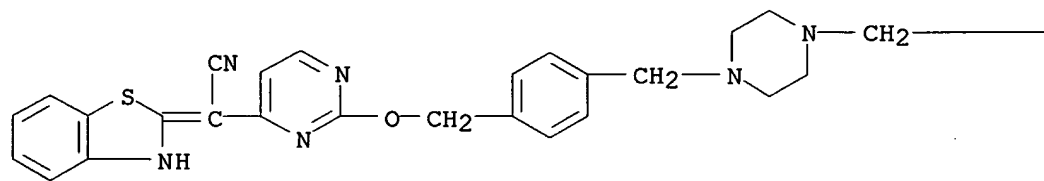
CN 1-Piperazinecarboxylic acid, 4-[[4-[[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy)methyl]phenyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)



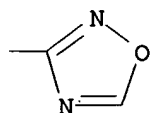
RN 622381-57-1 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[4-[[4-(1,2,4-oxadiazol-3-ylmethyl)-1-piperazinyl]methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)

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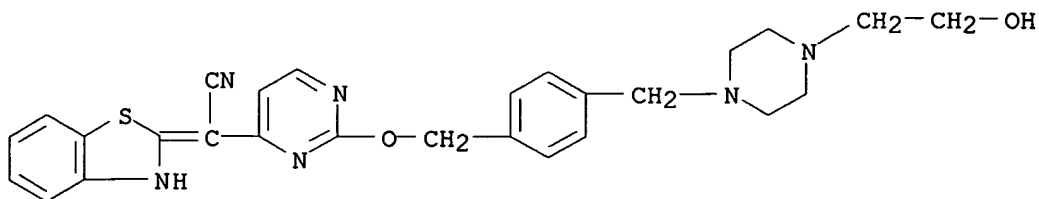


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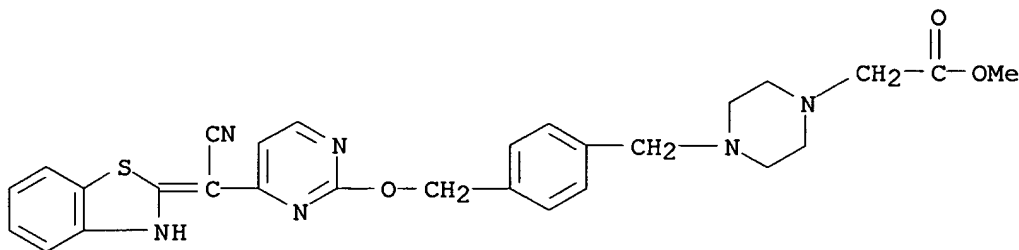
RN 622381-59-3 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[4-[[4-(2-hydroxyethyl)-1-piperazinyl]methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)



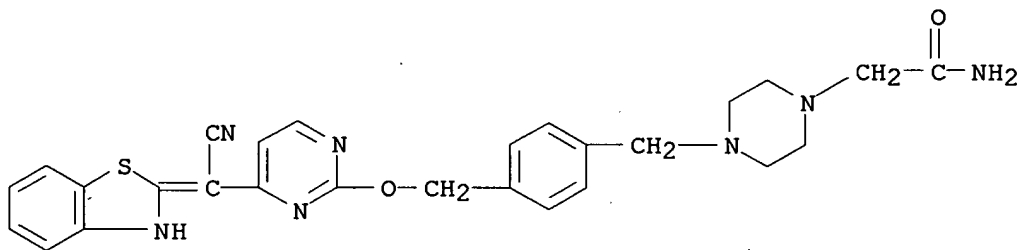
RN 622381-61-7 CAPLUS

CN 1-Piperazineacetic acid, 4-[[4-[[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)



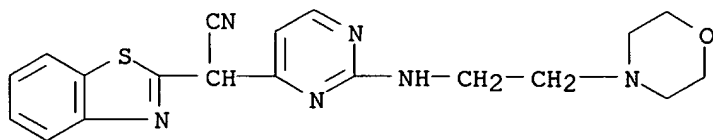
RN 622381-63-9 CAPLUS

CN 1-Piperazineacetamide, 4-[[4-[[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



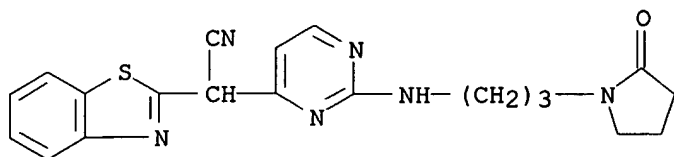
RN 848343-80-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, alpha-[2-[[2-(4-morpholinyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



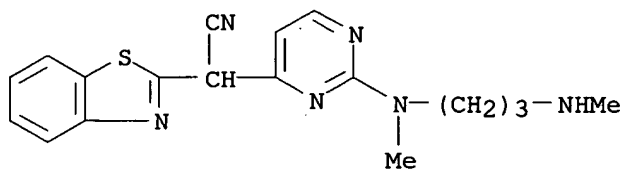
RN 848343-82-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, alpha-[2-[[3-(2-oxo-1-pyrrolidinyl)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



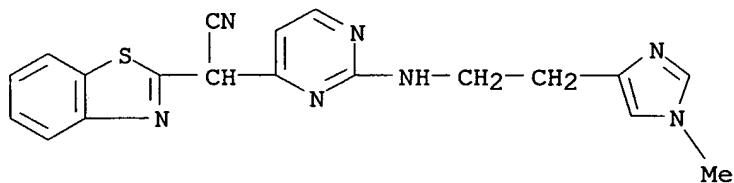
RN 848343-83-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[methyl[3-(methylamino)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



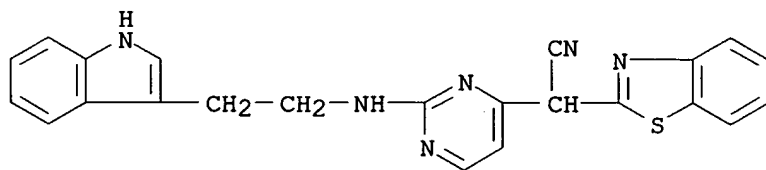
RN 848343-86-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[2-(1-methyl-1H-imidazol-4-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



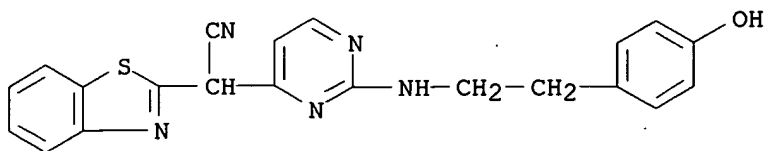
RN 848343-87-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[2-(1H-indol-3-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



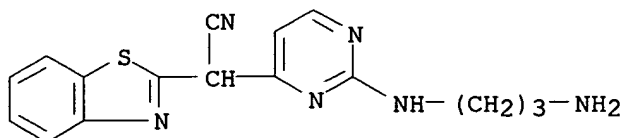
RN 848343-88-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



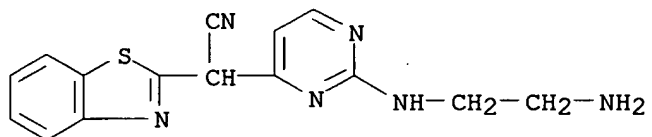
RN 848343-90-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(3-aminopropyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



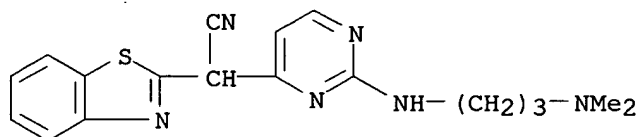
RN 848343-91-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-aminoethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



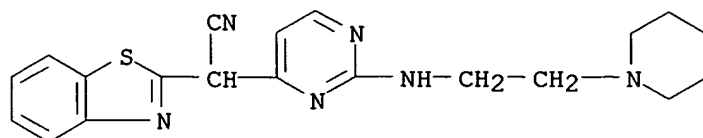
RN 848343-92-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(dimethylamino)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 848343-93-1 CAPLUS

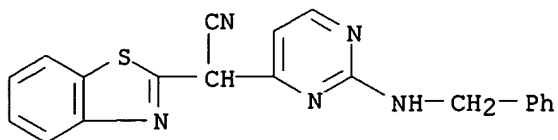
CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(1-piperidinyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 848343-94-2 CAPLUS

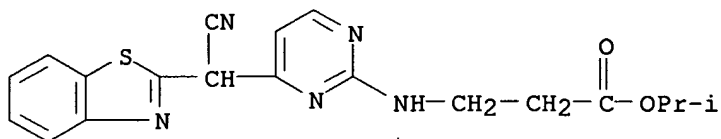
CN 2-Benzothiazoleacetonitrile, α-[2-[(phenylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

pyrimidinyl]- (9CI) (CA INDEX NAME)



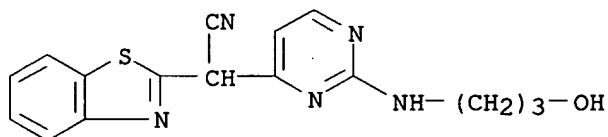
RN 848343-95-3 CAPLUS

CN  $\beta$ -Alanine, N-[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)



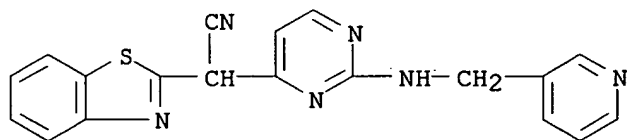
RN 848343-96-4 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[(3-hydroxypropyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



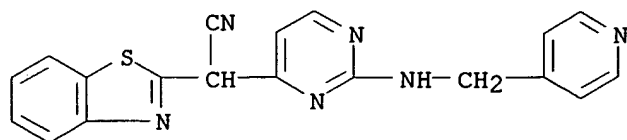
RN 848343-97-5 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[(3-pyridinylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

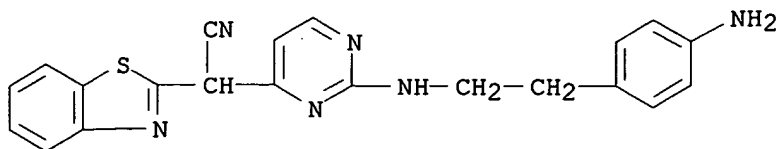


RN 848343-98-6 CAPLUS

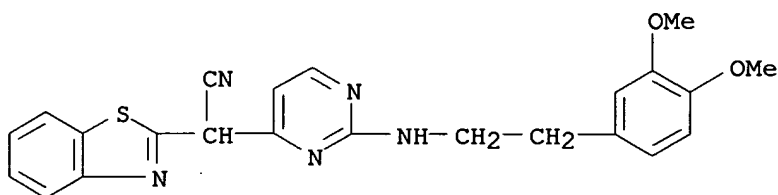
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[(4-pyridinylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



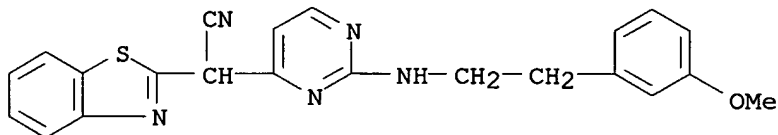
RN 848344-00-3 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(4-aminophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

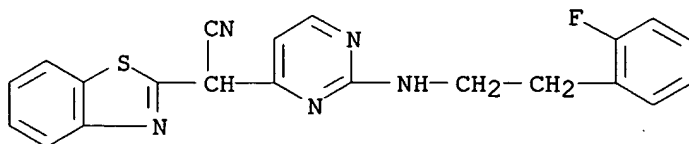
RN 848344-01-4 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-02-5 CAPLUS

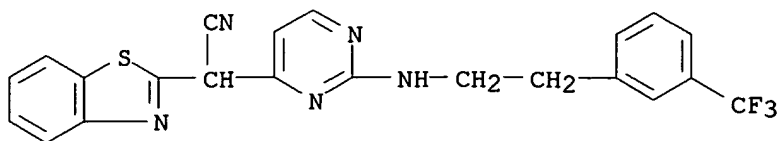
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(3-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-03-6 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(2-fluorophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

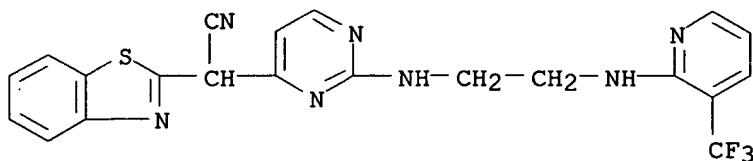
RN 848344-04-7 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-[3-(trifluoromethyl)phenyl]ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



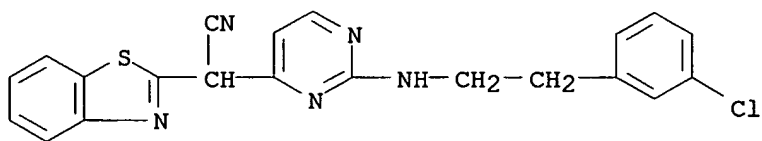
RN 848344-06-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-[[3-(trifluoromethyl)-2-pyridinyl]amino]ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



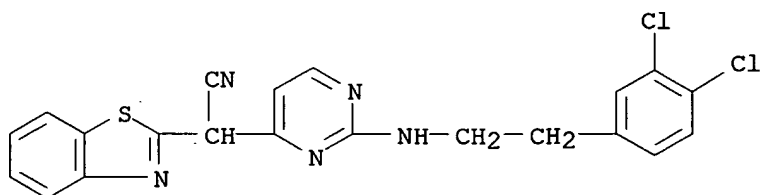
RN 848344-07-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3-chlorophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



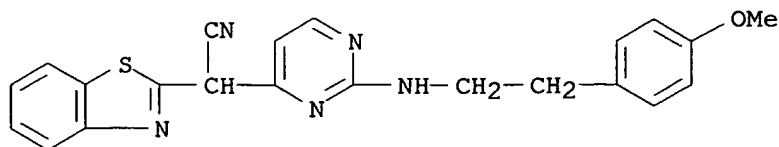
RN 848344-08-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3,4-dichlorophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



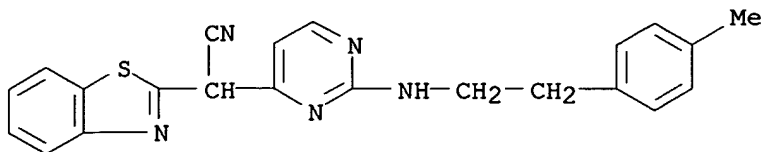
RN 848344-09-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

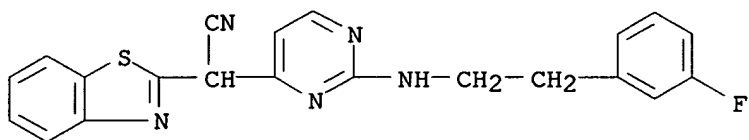




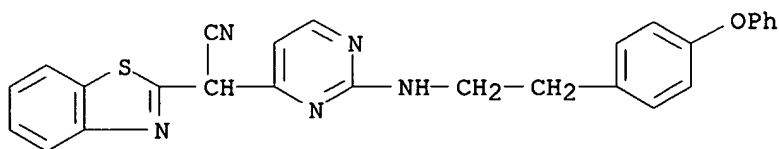
RN 848344-10-5 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[2-(4-methylphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

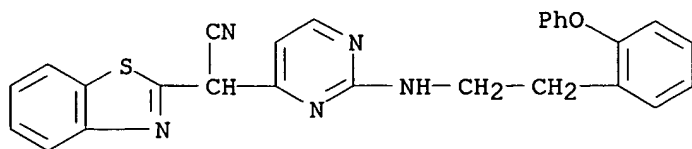
RN 848344-11-6 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[2-(3-fluorophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-12-7 CAPLUS

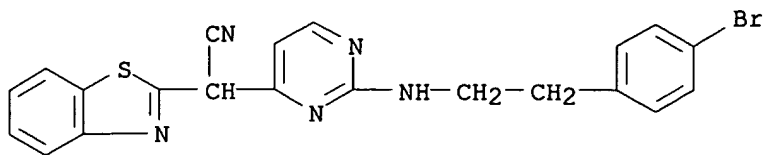
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[2-(4-phenoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-13-8 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[2-(2-phenoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

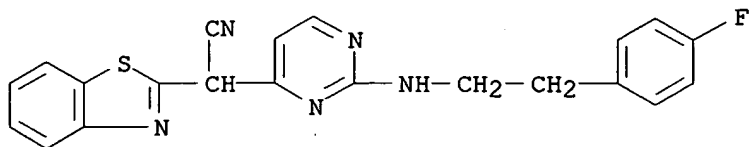
RN 848344-14-9 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[2-(4-bromophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



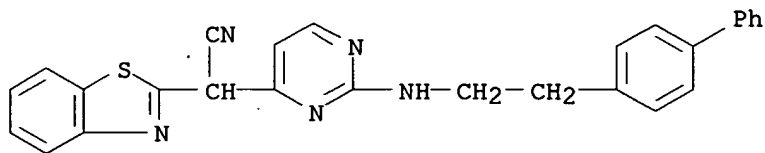
RN 848344-15-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(4-fluorophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



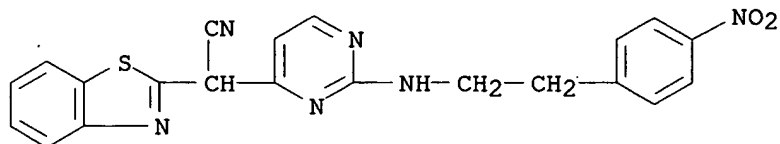
RN 848344-16-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-[1,1'-biphenyl]-4-ylethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



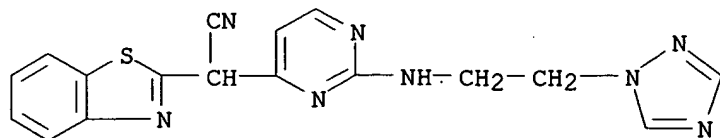
RN 848344-17-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(4-nitrophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 848344-18-3 CAPLUS

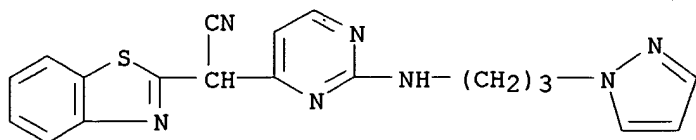
CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(1H-1,2,4-triazol-1-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 848344-19-4 CAPLUS

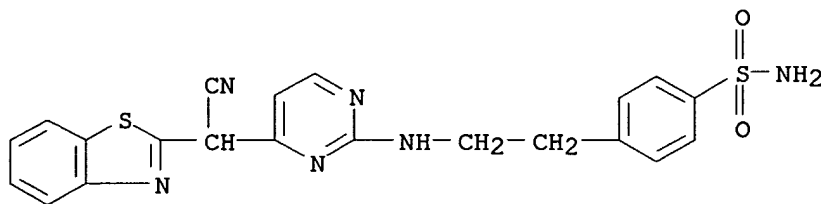
CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(1H-pyrazol-1-yl)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

4-pyrimidinyl]- (9CI) (CA INDEX NAME)

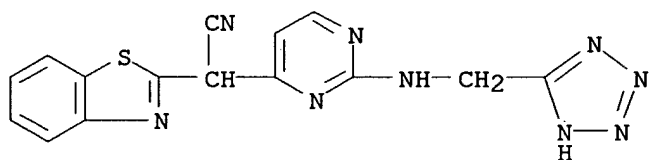


RN 848344-20-7 CAPLUS

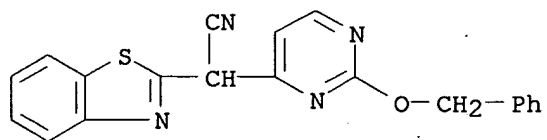
CN Benzenesulfonamide, 4-[2-[[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)



RN 848344-22-9 CAPLUS

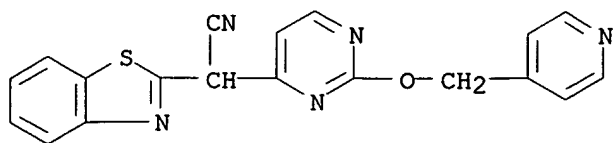
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[(1H-tetrazol-5-ylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-23-0 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(phenylmethoxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

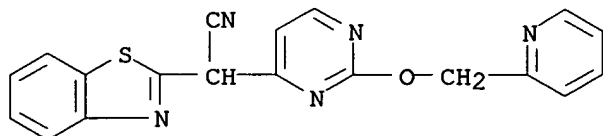
RN 848344-25-2 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(4-pyridinylmethoxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



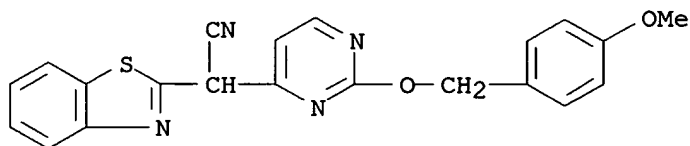
RN 848344-26-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(2-pyridinylmethoxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



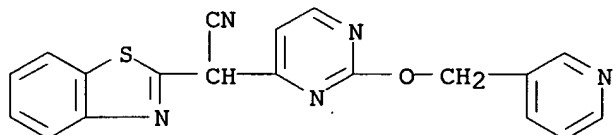
RN 848344-28-5 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(4-methoxyphenyl)methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



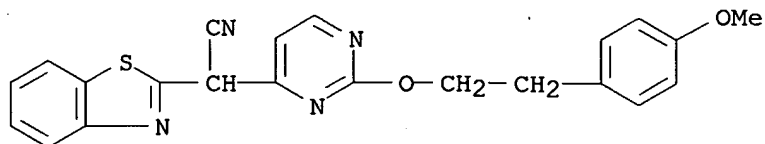
RN 848344-29-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(3-pyridinylmethoxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 848344-30-9 CAPLUS

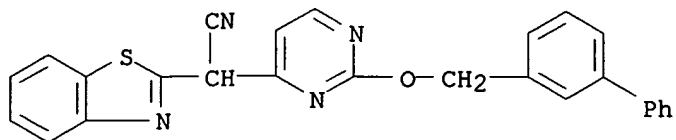
CN 2-Benzothiazoleacetonitrile, α-[2-[2-(4-methoxyphenyl)ethoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 848344-31-0 CAPLUS

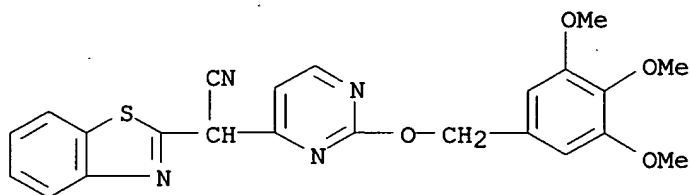
CN 2-Benzothiazoleacetonitrile, α-[2-([1,1'-biphenyl]-3-ylmethoxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

pyrimidinyl]- (9CI) (CA INDEX NAME)



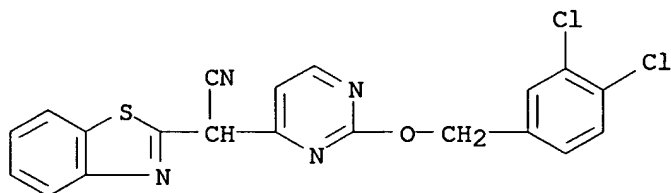
RN 848344-32-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(3,4,5-trimethoxyphenyl)methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



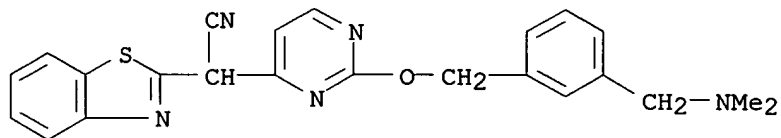
RN 848344-33-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(3,4-dichlorophenyl)methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



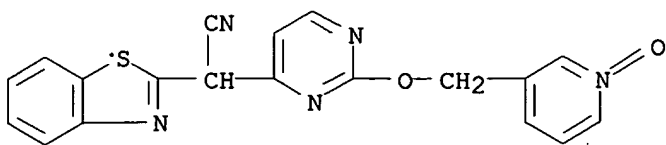
RN 848344-34-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-[(dimethylamino)methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



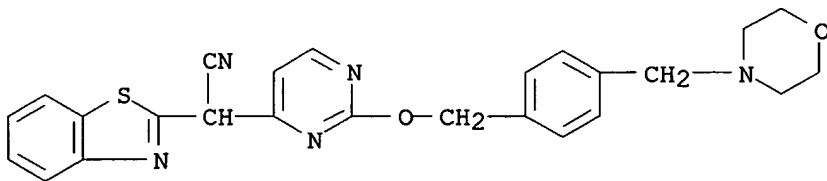
RN 848344-35-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(1-oxido-3-pyridinyl)methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



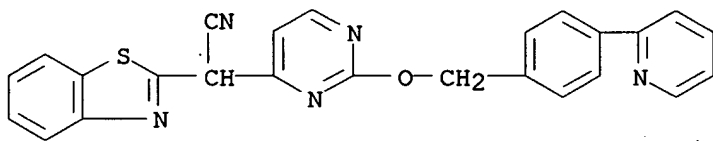
RN 848344-36-5 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(4-morpholinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



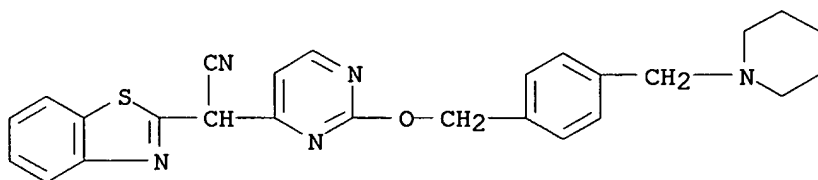
RN 848344-37-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(2-pyridinyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



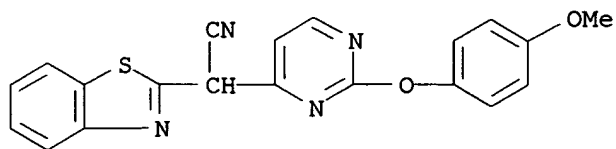
RN 848344-38-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(1-piperidinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

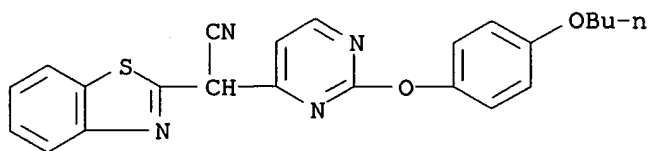


RN 848344-39-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(4-methoxyphenoxy)-4-pyrimidinyl]-2-morpholinylmethyl]phenylmethoxy-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

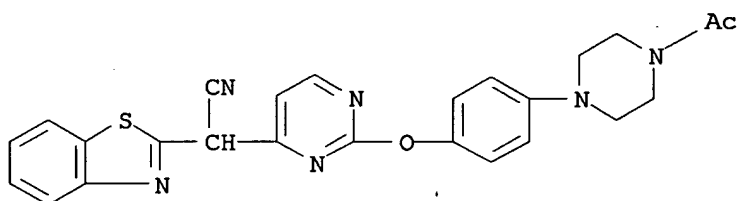


RN 848344-40-1 CAPLUS

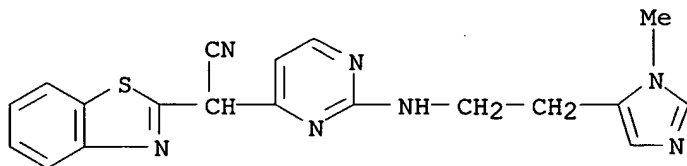
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(4-butoxyphenoxy)-4-pyrimidinyl]-  
(9CI) (CA INDEX NAME)

RN 848344-41-2 CAPLUS

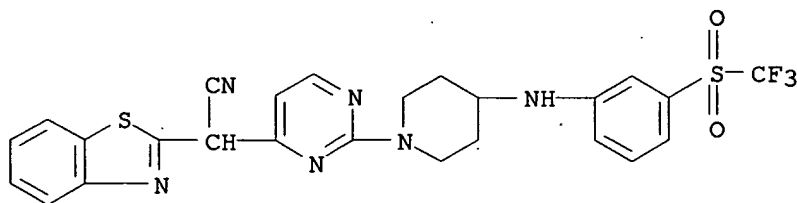
CN Piperazine, 1-acetyl-4-[4-[[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]oxy]phenyl]- (9CI) (CA INDEX NAME)



RN 848344-70-7 CAPLUS

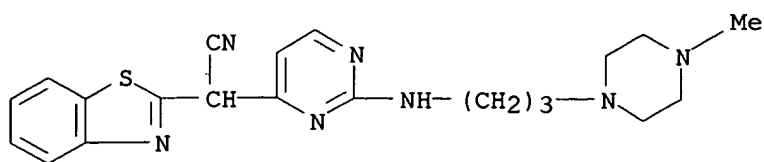
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(1-methyl-1H-imidazol-5-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 866916-11-2 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[4-[[3-[(trifluoromethyl)sulfonyl]phenyl]amino]-1-piperidinyl]-4-pyrimidinyl]-  
(9CI) (CA INDEX NAME)

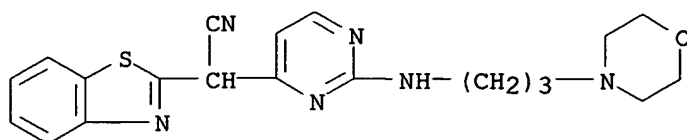
RN 866916-12-3 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[3-(4-methyl-1-piperazinyl)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



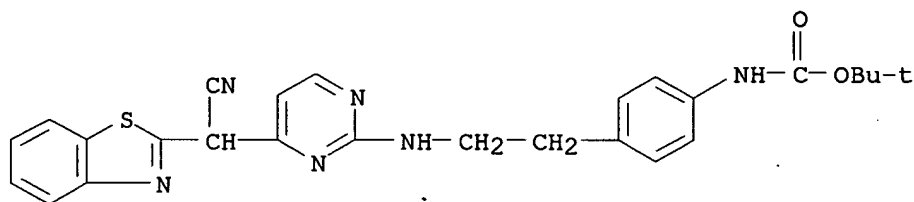
RN 866916-13-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(4-morpholinyl)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



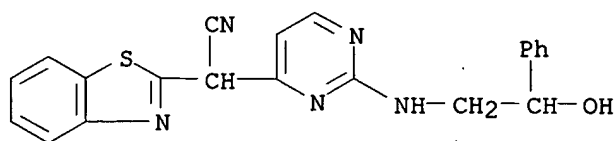
RN 866916-14-5 CAPLUS

CN Carbamic acid, [4-[2-[[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]amino]ethyl]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 866916-15-6 CAPLUS

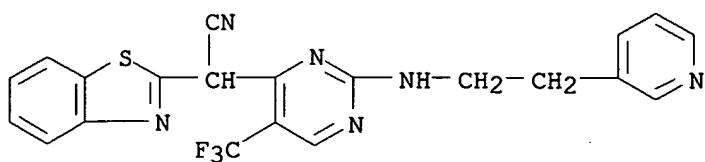
CN 2-Benzothiazoleacetonitrile, α-[2-[(2-hydroxy-2-phenylethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 866916-17-8 CAPLUS

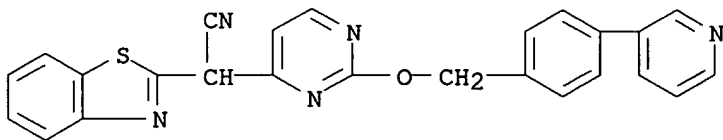
CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3-pyridinyl)ethyl]amino]-5-(trifluoromethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)





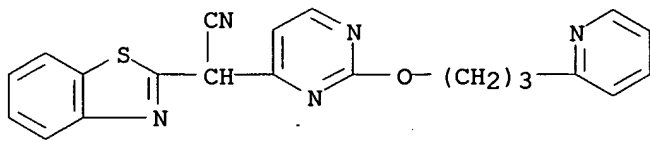
RN 866916-18-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(3-pyridinyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



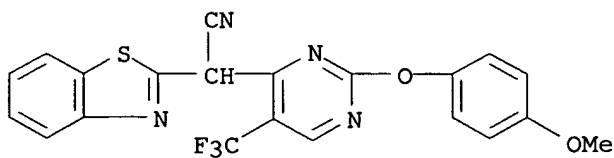
RN 866916-19-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[3-(2-pyridinyl)propoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



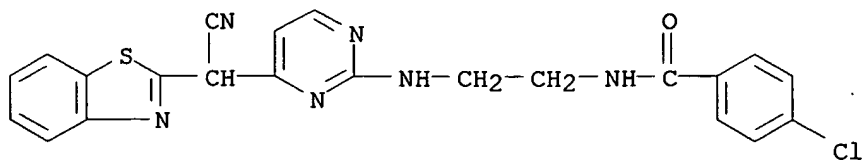
RN 866916-20-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(4-methoxyphenoxy)-5-(trifluoromethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



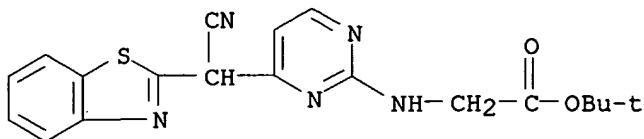
RN 866916-21-4 CAPLUS

CN Benzamide, N-[2-[[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]amino]ethyl]-4-chloro- (9CI) (CA INDEX NAME)



RN 866916-22-5 CAPLUS

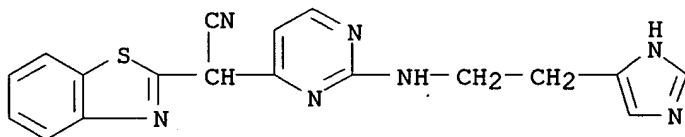
CN Glycine, N-[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



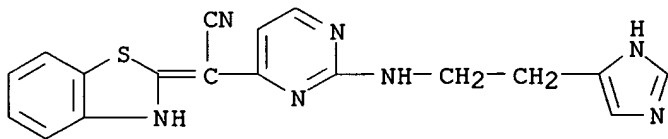
IT 345986-64-3

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(pharmaceutical composition comprising JNK inhibitor and cyclosporin)

RN 345986-64-3 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[2-(1H-imidazol-4-yl)ethyl]amino]-4-pyrimidinyl- (9CI) (CA INDEX NAME)RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

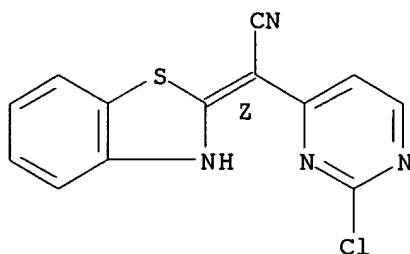
L4 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2005:1059107 CAPLUS  
 DN 143:472316  
 TI Anatomy of Fingerprint Search Calculations on Structurally Diverse Sets of Active Compounds  
 AU Godden, Jeffrey W.; Stahura, Florence L.; Bajorath, Juergen  
 CS Department of Life Science Informatics, Rheinische Friedrich-Wilhelms-Universitaet, Bonn, D-53113, Germany  
 SO Journal of Chemical Information and Modeling (2005), 45(6), 1812-1819  
 CODEN: JCISD8; ISSN: 1549-9596  
 PB American Chemical Society  
 DT Journal  
 LA English  
 AB Similarity searching using mol. fingerprints is a widely used approach for the identification of novel hits. A fingerprint search involves many pairwise comparisons of bit string representations of known active mols. with those precomputed for database compds. Bit string overlap, as evaluated by various similarity metrics, is used as a measure of mol. similarity. Results of a number of studies focusing on fingerprints suggest that it is difficult, if not impossible, to develop generally applicable search parameters and strategies, irresp. of the compound classes under investigation. Rather, more or less, each individual search problem requires an adjustment of calcn. conditions. Thus, there is a need for diagnostic tools to analyze fingerprint-based similarity searching. The authors report an anal. of fingerprint search calcns. on different sets of structurally diverse active compds. Calcns. on five biol. activity classes were carried out with two fingerprints in two compound source databases, and the results were analyzed in histograms. Tanimoto coefficient (Tc) value ranges where active compds. were detected were compared to the distribution of Tc values in the database. The anal. revealed that compound class-specific effects strongly influenced the outcome of these fingerprint calcns. Among the five diverse compound sets studied, very different search results were obtained. The anal. described here can be applied to determine Tc intervals where scaffold hopping occurs. It can also be used to benchmark fingerprint calcns. or estimate their probability of success.  
 IT 869584-23-6  
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (fingerprint search calcns. on structurally diverse sets of active compds.)  
 RN 869584-23-6 CAPLUS  
 CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(1H-imidazol-4-yl)ethyl]amino]- (9CI) (CA INDEX NAME)



RE.CNT 88 THERE ARE 88 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2005:485713 CAPLUS  
 DN 143:172830  
 TI Design and Synthesis of the First Generation of Novel Potent, Selective, and in Vivo Active (Benzothiazol-2-yl)acetonitrile Inhibitors of the c-Jun N-Terminal Kinase  
 AU Gaillard, Pascale; Jeanclaude-Etter, Isabelle; Ardisson, Vittoria; Arkinstall, Steve; Cambet, Yves; Camps, Montserrat; Chabert, Christian; Church, Dennis; Cirillo, Rocco; Gretener, Denise; Halazy, Serge; Nichols, Anthony; Szyndralewicz, Cedric; Vitte, Pierre-Alain; Gotteland, Jean-Pierre  
 CS SeroPharmaceutical Research Institute, Geneva, 1228, Switz.  
 SO Journal of Medicinal Chemistry (2005), 48(14), 4596-4607  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PB American Chemical Society  
 DT Journal  
 LA English  
 OS CASREACT 143:172830  
 AB Several lines of evidence support the hypothesis that c-Jun N-terminal kinase (JNKs) plays a critical role in a wide range of diseases including cell death (apoptosis)-related disorders (neurodegenerative diseases, brain, heart, and renal ischemia, epilepsy) and inflammatory disorders (multiple sclerosis, rheumatoid arthritis, inflammatory bowel diseases). Screening of an internal compound collection for inhibitors of JNK3 led to the identification of (benzothiazol-2-yl)acetonitrile derivs. as potent and selective JNK1, -2, -3 inhibitors. Starting from initial hit I [R = Cl, R1 = Br] (AS007149), the chemical and initial structure-activity relationship (SAR) of this novel and unique kinase inhibitor template were explored. Investigation of the SAR rapidly revealed that the benzothiazol-2-ylacetonitrile pyrimidine core was crucial to retain a good level of potency on rat JNK3. Therefore, I [R = Cl, R1 = H] was further optimized by exploring a number of distal combinations in place of the chlorine atom. This led to the observation that the presence of an aromatic group, two carbons away from the aminopyrimidine moiety and bearing substituents conferring hydrogen bond acceptor (HBA) properties, could improve the potency. Further improvements to the biol. and biopharmaceutical profile of the most promising compds. were performed, resulting in the discovery of I [R = 2-(3-pyridinyl)ethyl, R1 = H] (AS601245). The in vitro and in vivo anti-inflammatory potential of this new JNK inhibitor was investigated and found to demonstrate efficacy per oral route in an exptl. model of rheumatoid arthritis (RA).  
 IT 861411-30-5P  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)  
 (design and synthesis of novel potent, selective, and in vivo active (benzothiazol-2-yl)acetonitrile inhibitors of the c-Jun N-terminal kinase)  
 RN 861411-30-5 CAPLUS  
 CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-chloro-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



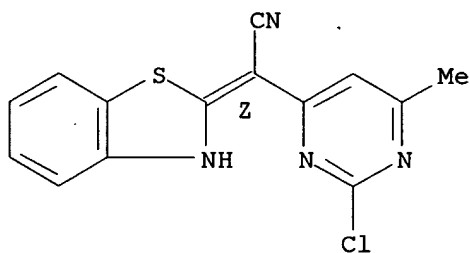
IT 861411-31-6P 861411-33-8P 861411-35-0P  
 861411-36-1P 861411-37-2P 861411-38-3P  
 861411-39-4P 861411-40-7P 861411-41-8P  
 861411-42-9P 861411-43-0P 861411-44-1P  
 861411-45-2P 861411-46-3P 861411-47-4P  
 861411-48-5P 861411-49-6P 861411-50-9P  
 861411-51-0P 861411-52-1P 861411-53-2P  
 861411-54-3P 861411-55-4P 861411-56-5P  
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 861411-72-5P 861411-73-6P 861411-74-7P  
 861411-75-8P 861411-76-9P 861411-77-0P  
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL  
 (Biological study); PREP (Preparation)  
 (design and synthesis of novel potent, selective, and in vivo active  
 (benzothiazol-2-yl)acetonitrile inhibitors of the c-Jun N-terminal  
 kinase)

RN 861411-31-6 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-chloro-6-  
 methyl-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

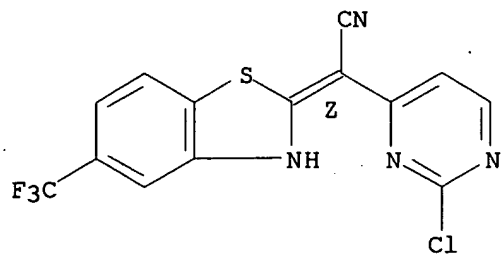
Double bond geometry as shown.



RN 861411-33-8 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-chloro- $\alpha$ -[5-(trifluoromethyl)-2(3H)-  
 benzothiazolylidene]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

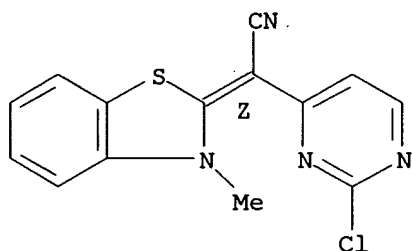
Double bond geometry as shown.



RN 861411-35-0 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-chloro- $\alpha$ -(3-methyl-2(3H)-benzothiazolylidene)-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

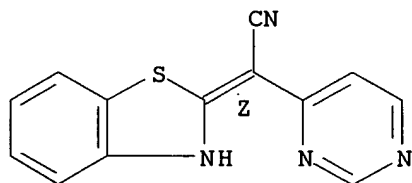
Double bond geometry as shown.



RN 861411-36-1 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

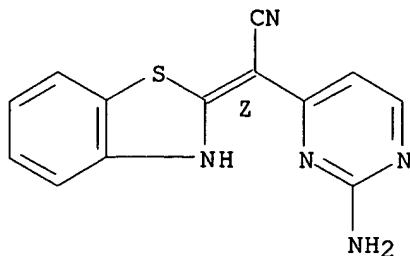
Double bond geometry as shown.



RN 861411-37-2 CAPLUS

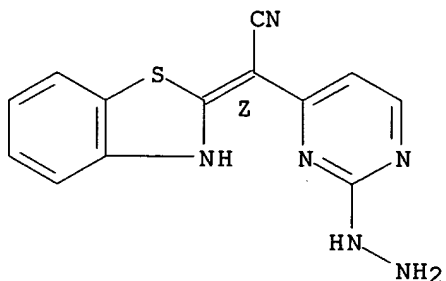
CN 4-Pyrimidineacetonitrile, 2-amino- $\alpha$ -2(3H)-benzothiazolylidene-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



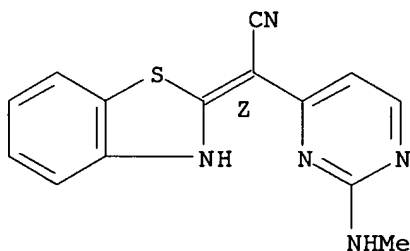
RN 861411-38-3 CAPLUS  
 CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-hydrazino-,  
 ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



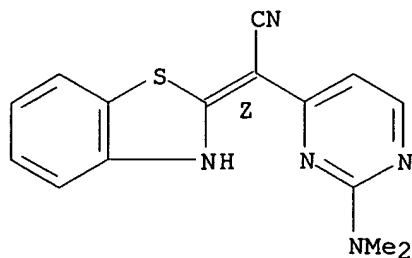
RN 861411-39-4 CAPLUS  
 CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-(methylamino)-,  
 ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 861411-40-7 CAPLUS  
 CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-(dimethylamino)-,  
 ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

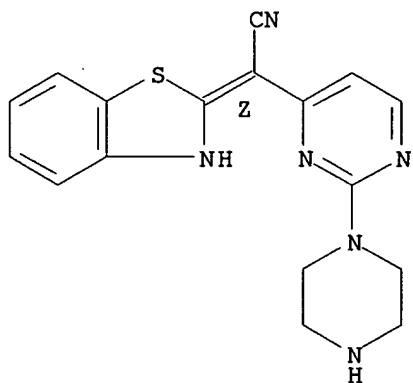
Double bond geometry as shown.



RN 861411-41-8 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-(1-piperazinyl)-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

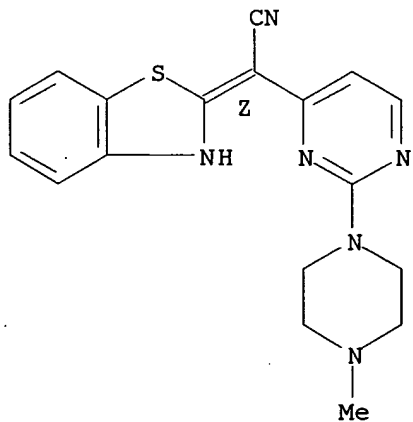
Double bond geometry as shown.



RN 861411-42-9 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-(4-methyl-1-piperazinyl)-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

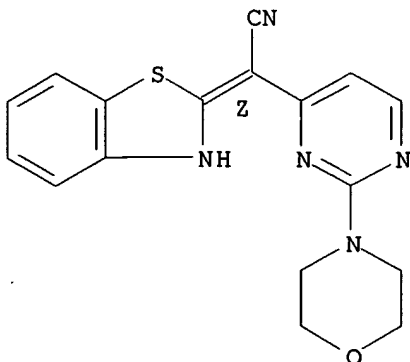


RN 861411-43-0 CAPLUS



CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-(4-morpholinyl)-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

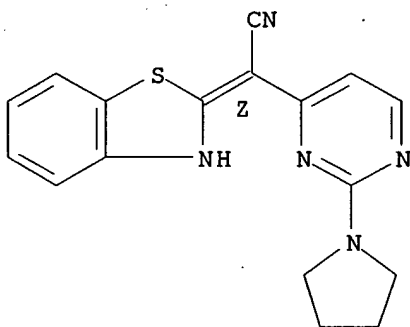
Double bond geometry as shown.



RN 861411-44-1 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-(1-pyrrolidinyl)-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

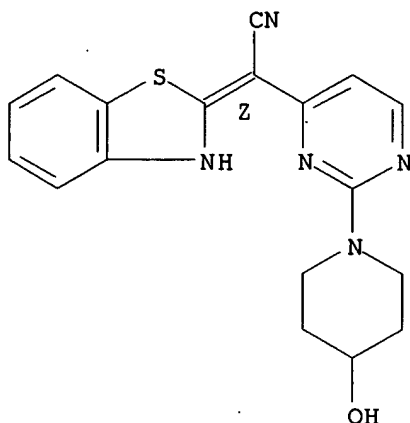
Double bond geometry as shown.



RN 861411-45-2 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-(4-hydroxy-1-piperidinyl)-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

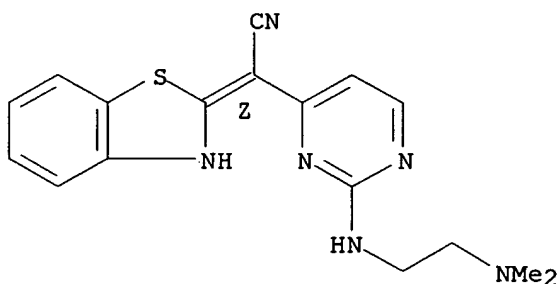
Double bond geometry as shown.



RN 861411-46-3 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(dimethylamino)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

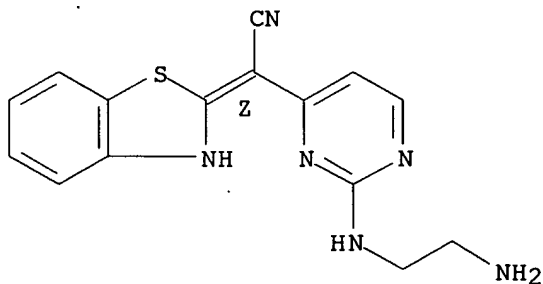
Double bond geometry as shown.



RN 861411-47-4 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-[(2-aminoethyl)amino]- $\alpha$ -2(3H)-benzothiazolylidene-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

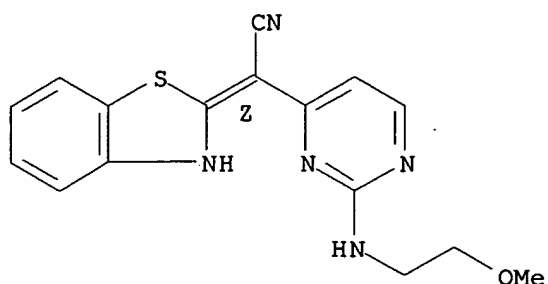
Double bond geometry as shown.



RN 861411-48-5 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[(2-methoxyethyl)amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

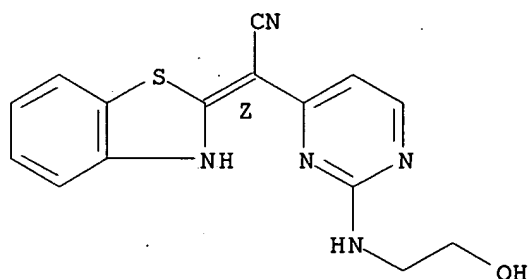
Double bond geometry as shown.



RN 861411-49-6 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylden-2-[(2-hydroxyethyl)amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

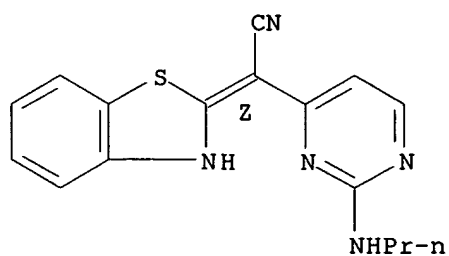
Double bond geometry as shown.



RN 861411-50-9 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolydene-2-(propylamino)-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

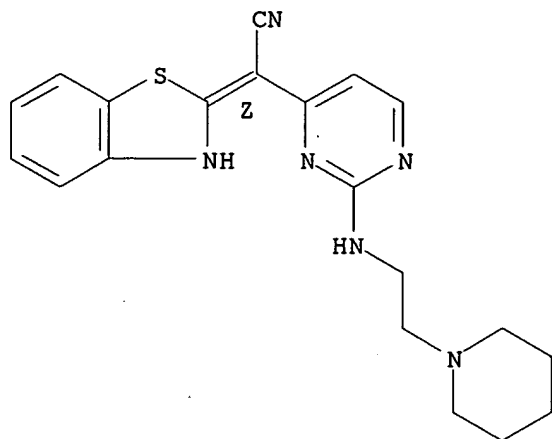
Double bond geometry as shown.



RN 861411-51-0 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylden-2-[[2-(1-piperidinyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

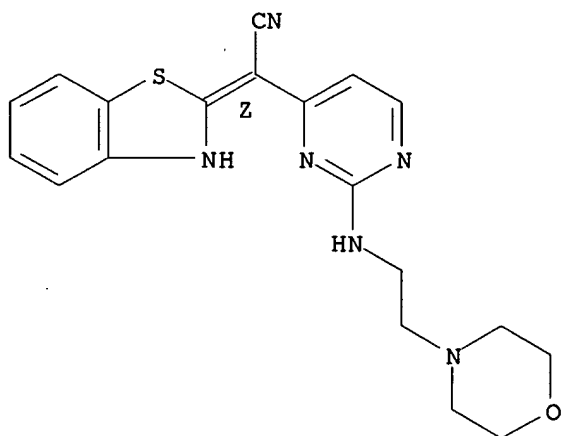
Double bond geometry as shown.



RN 861411-52-1 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(4-morpholinyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

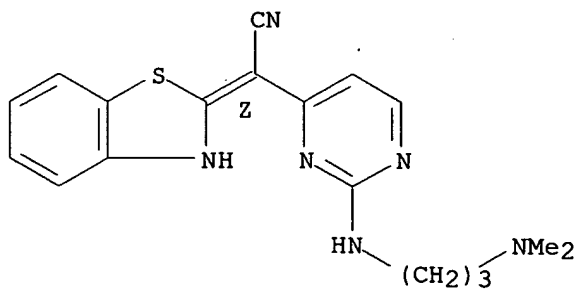
Double bond geometry as shown.



RN 861411-53-2 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[3-(dimethylamino)propyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

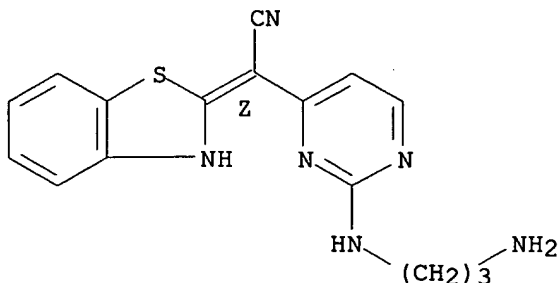
Double bond geometry as shown.



RN 861411-54-3 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-[(3-aminopropyl)amino]- $\alpha$ -2(3H)-benzothiazolylidene-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

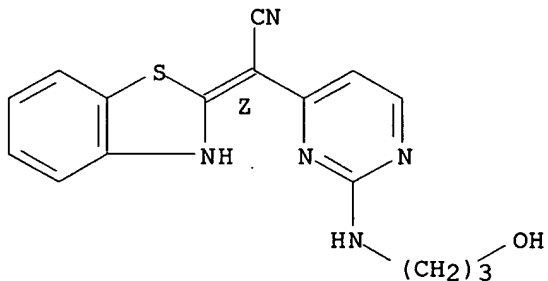
Double bond geometry as shown.



RN 861411-55-4 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[(3-hydroxypropyl)amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

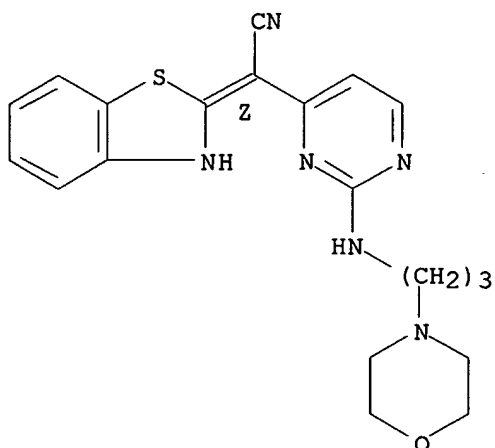
Double bond geometry as shown.



RN 861411-56-5 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[3-(4-morpholinyl)propyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

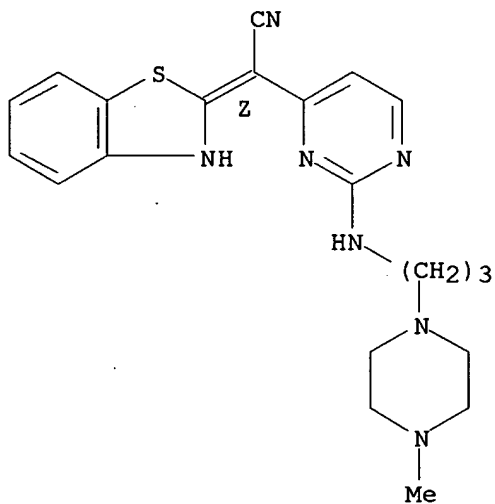
Double bond geometry as shown.



RN 861411-57-6 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[3-(4-methyl-1-piperazinyl)propyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

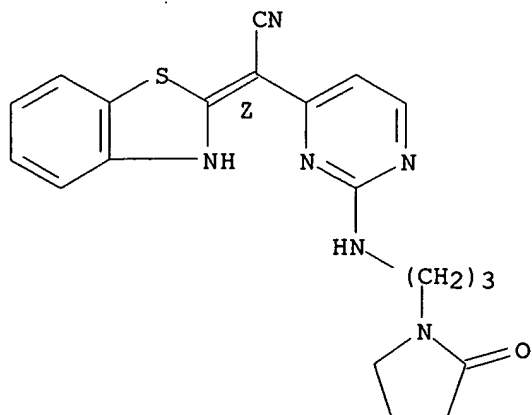
Double bond geometry as shown.



RN 861411-58-7 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[3-(2-oxo-1-pyrrolidiny)propyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

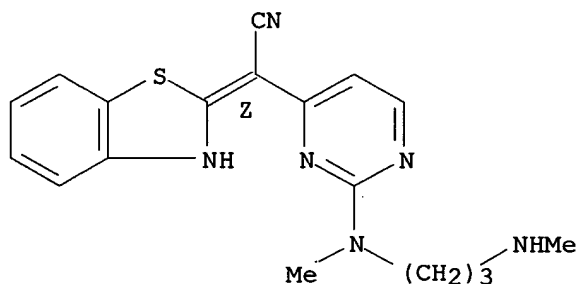
Double bond geometry as shown.



RN 861411-59-8 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[methyl[3-(methylamino)propyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

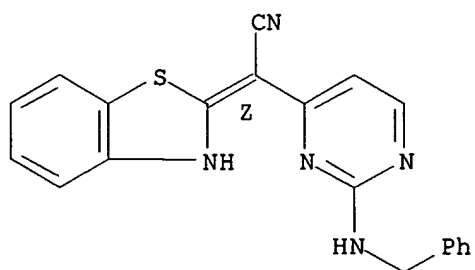
Double bond geometry as shown.



RN 861411-60-1 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[(phenylmethyl)amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

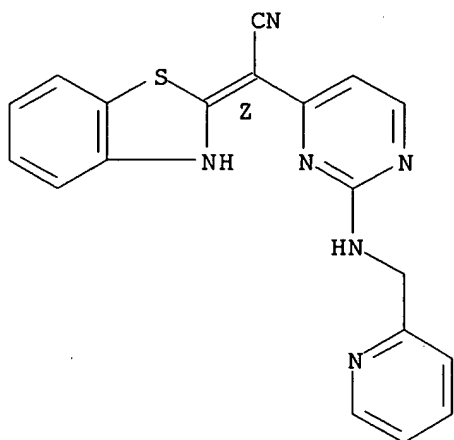
Double bond geometry as shown.



RN 861411-61-2 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[(2-pyridinylmethyl)amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

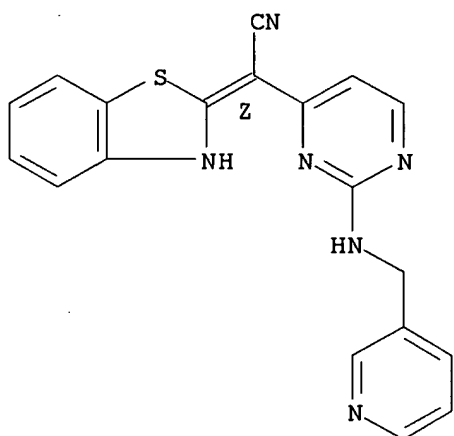
Double bond geometry as shown.



RN 861411-62-3 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[(3-pyridinylmethyl)amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

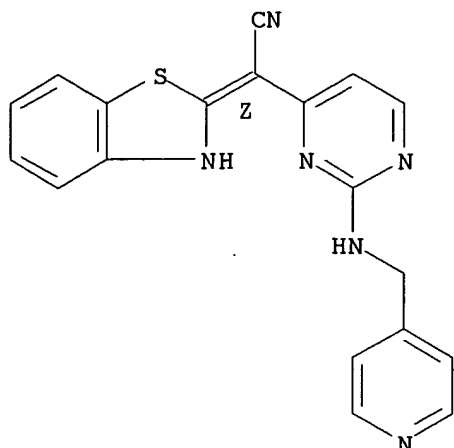


RN 861411-63-4 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[(4-pyridinylmethyl)amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

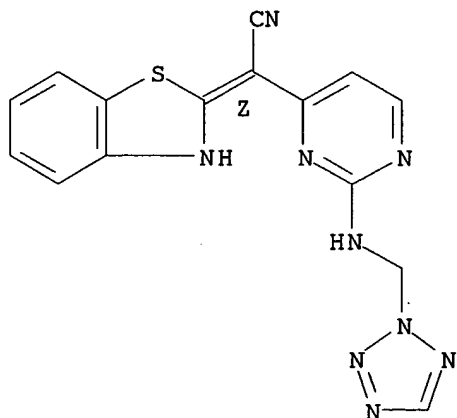




RN 861411-64-5 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[(2H-tetrazol-2-ylmethyl)amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

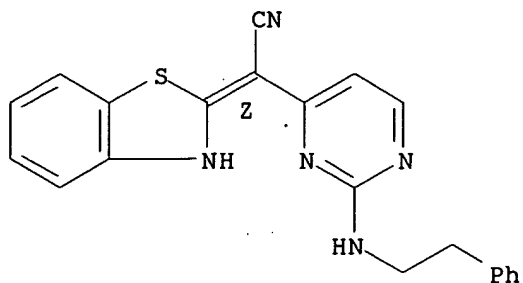
Double bond geometry as shown.



RN 861411-65-6 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[(2-phenylethyl)amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

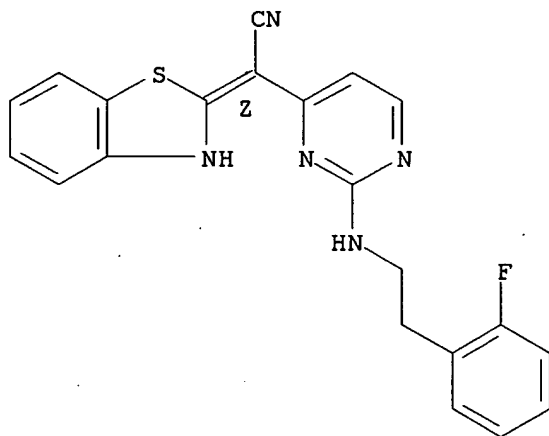
Double bond geometry as shown.



RN 861411-66-7 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(2-fluorophenyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

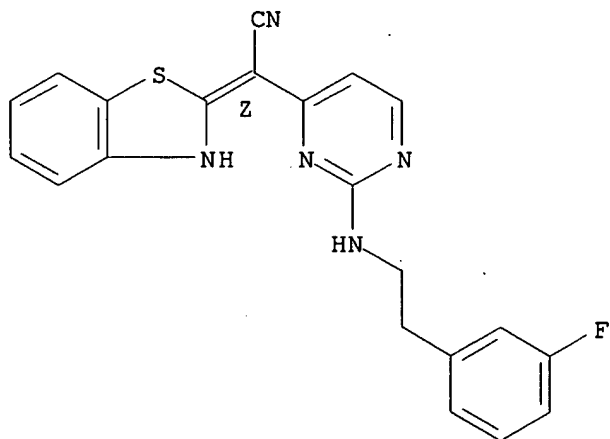
Double bond geometry as shown.



RN 861411-67-8 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(3-fluorophenyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

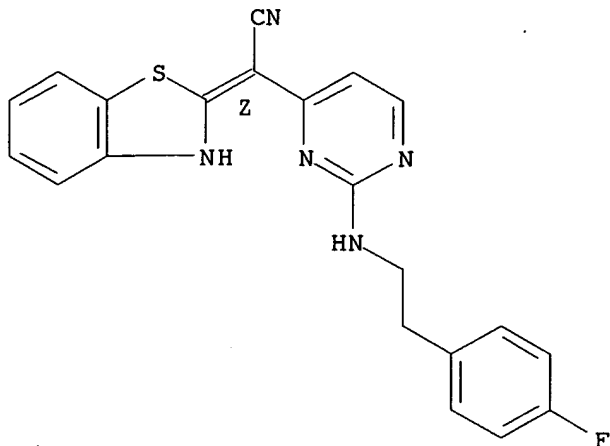
Double bond geometry as shown.



RN 861411-68-9 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(4-fluorophenyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

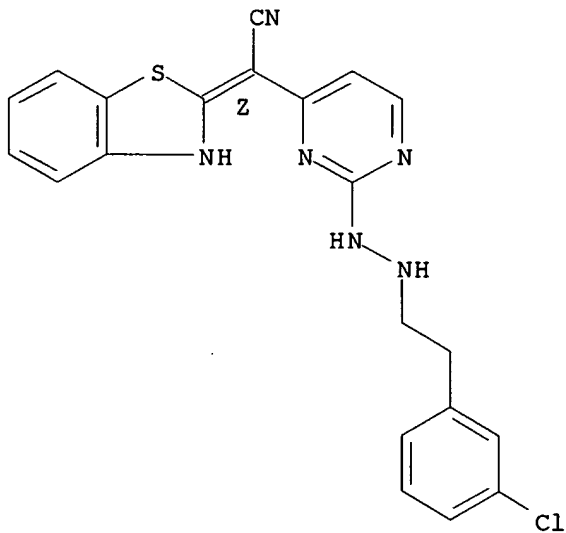
Double bond geometry as shown.



RN 861411-69-0 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[2-[2-(3-chlorophenyl)ethyl]hydrazino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

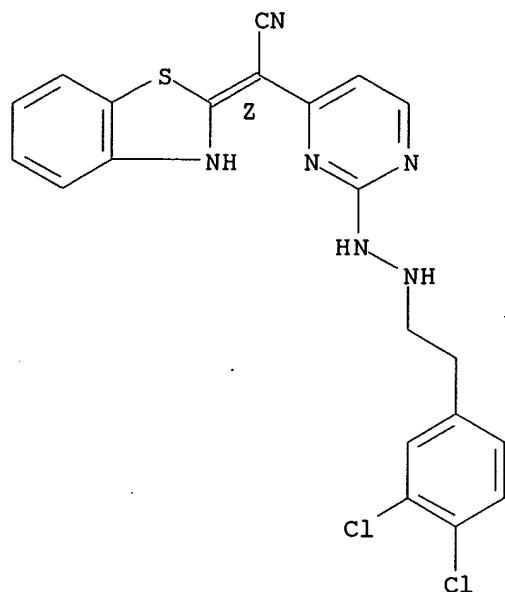
Double bond geometry as shown.



RN 861411-70-3 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[2-[2-(3,4-dichlorophenyl)ethyl]hydrazino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

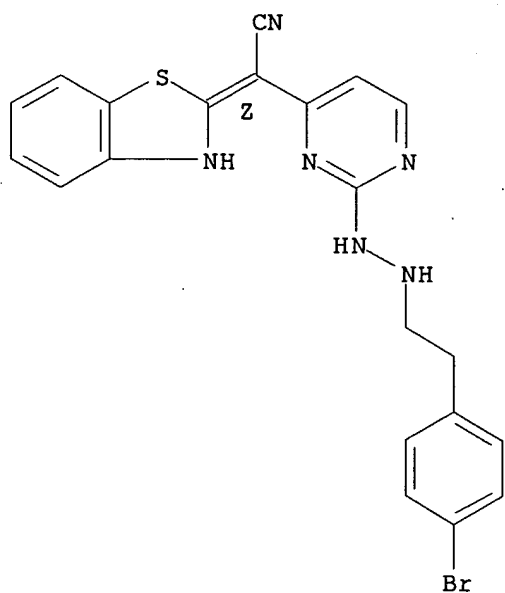
Double bond geometry as shown.



RN 861411-71-4 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[2-[2-(4-bromophenyl)ethyl]hydrazino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

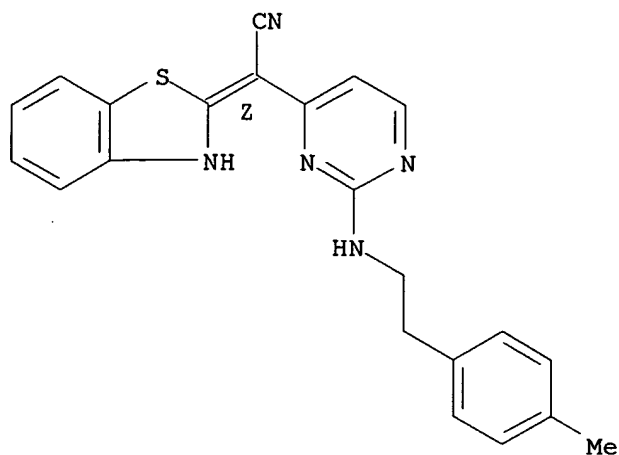
Double bond geometry as shown.



RN 861411-72-5 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(4-methylphenyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

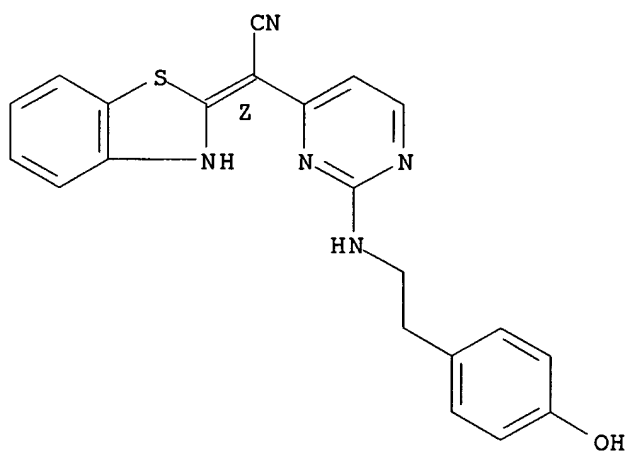
Double bond geometry as shown.



RN 861411-73-6 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(4-hydroxyphenyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

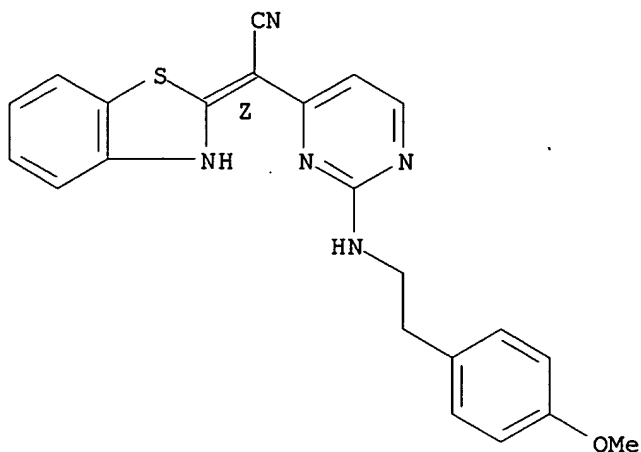
Double bond geometry as shown.



RN 861411-74-7 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(4-methoxyphenyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

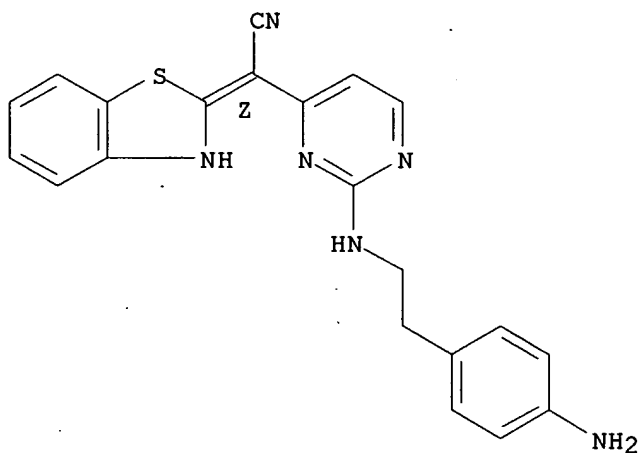
Double bond geometry as shown.



RN 861411-75-8 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-[[2-(4-aminophenyl)ethyl]amino]- $\alpha$ -2(3H)-benzothiazolylidene-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

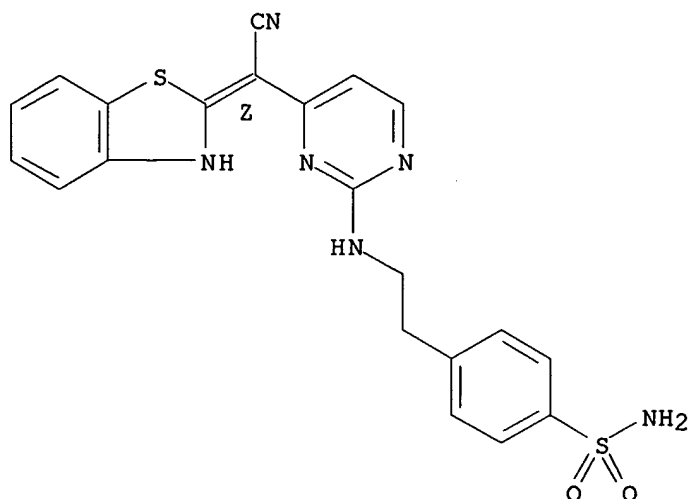
Double bond geometry as shown.



RN 861411-76-9 CAPLUS

CN Benzenesulfonamide, 4-[2-[[4-[(Z)-2(3H)-benzothiazolylidenecyanomethyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

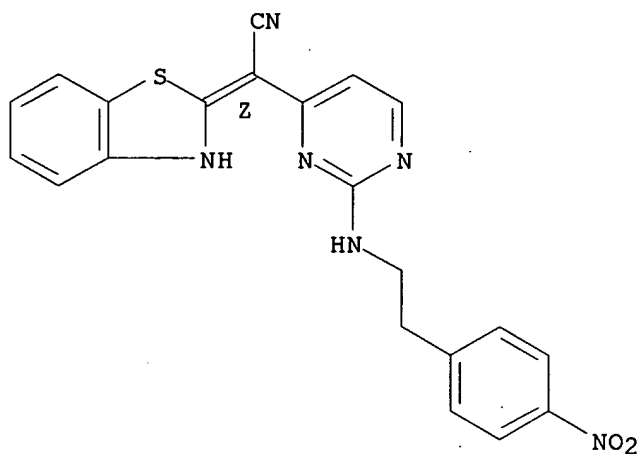
Double bond geometry as shown.



RN 861411-77-0 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(4-nitrophenyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

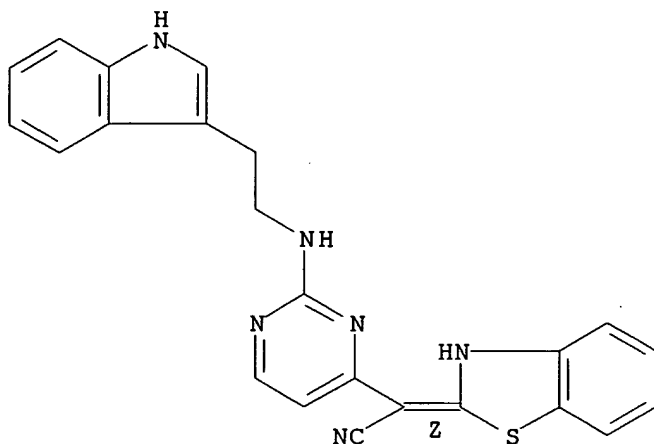
Double bond geometry as shown.



RN 861411-78-1 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(1H-indol-3-yl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

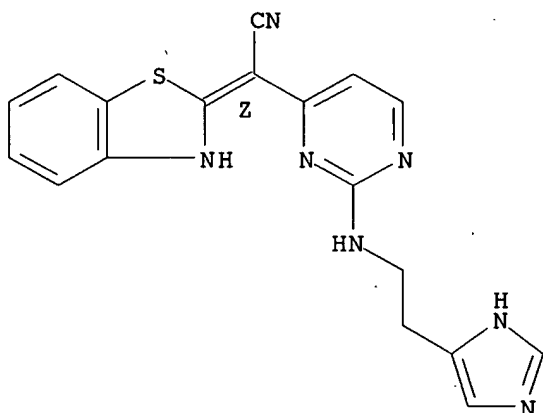
Double bond geometry as shown.



RN 861411-79-2 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(1H-imidazol-4-yl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

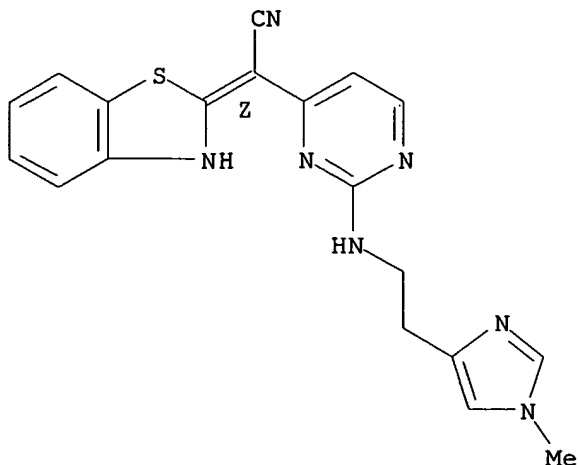


RN 861411-80-5 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(1-methyl-1H-imidazol-4-yl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

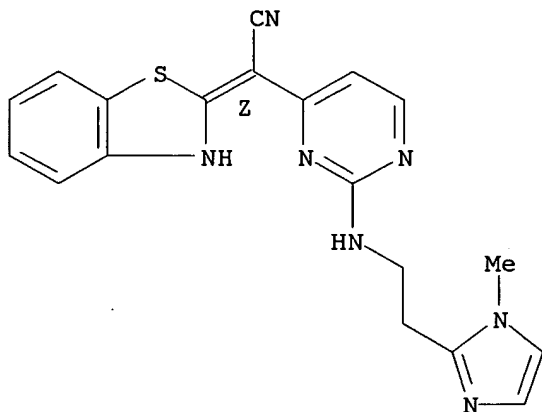




RN 861411-81-6 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(1-methyl-1H-imidazol-2-yl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

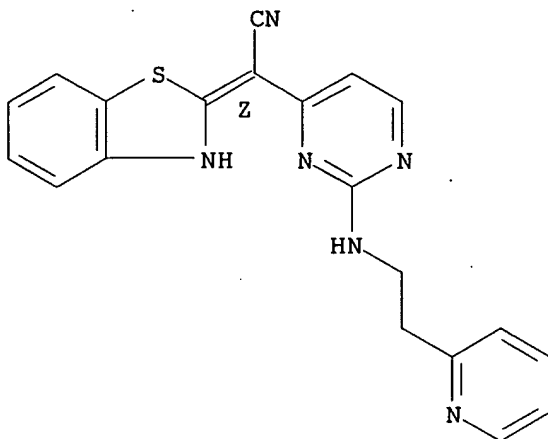
Double bond geometry as shown.



RN 861411-82-7 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(2-methylpyridin-2-yl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

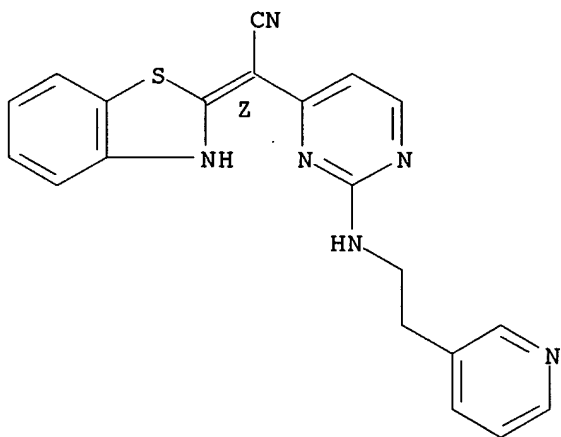
Double bond geometry as shown.



RN 861411-83-8 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(3-pyridinyl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

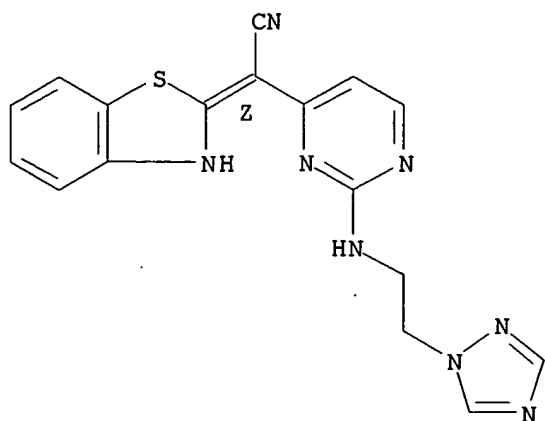
Double bond geometry as shown.



RN 861411-84-9 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[2-(1H-1,2,4-triazol-1-yl)ethyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

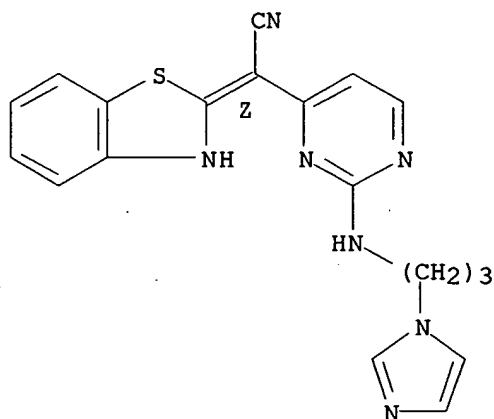
Double bond geometry as shown.



RN 861411-85-0 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[3-(1H-imidazol-1-yl)propyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

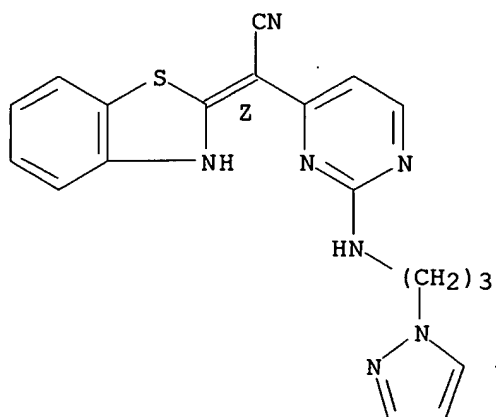
Double bond geometry as shown.



RN 861411-86-1 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[3-(1H-pyrazol-1-yl)propyl]amino]-, ( $\alpha$ Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2005:259876 CAPLUS

DN 142:341891

TI Benzothiazole derivatives for the treatment of diabetes

IN Gaillard, Pascale; Gotteland, Jean-Pierre; Vitte, Pierre-Alain

PA Applied Research Systems ARS Holding N.V., Neth. Antilles

SO PCT Int. Appl., 46 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005025567	A1	20050324	WO 2004-EP52090	20040908
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	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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	CA 2534314	AA	20050324	CA 2004-2534314	20040908
	EP 1696909	A1	20060906	EP 2004-787110	20040908
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	NO 2006001600	A	20060407	NO 2006-1600	20060407
PRAI	EP 2003-102740	A	20030912		
	WO 2004-EP52090	W	20040908		
OS	MARPAT 142:341891				
AB	The present invention is related to the use of benzothiazole derivs. for the manufacture of a medicament for the treatment of metabolic disorders mediated by insulin resistance or hyperglycemia, comprising diabetes type II, inadequate glucose tolerance, insulin resistance, obesity, polycystic ovary syndrome (PCOS) Formula I. G is an unsubstituted or substituted pyrimidinyl group. L is an unsubstituted or substituted C1-C6-alkoxy, or an amino group, or an unsubstituted or a substituted 3-8 membered heterocycloalkyl, containing at least one heteroatom selected from N, O, S (e.g. a piperazine, a piperidine, a morpholine, a pyrrolidine). R1 is selected from the group comprising or consisting of hydrogen, sulfonyl, amino, unsubstituted or substituted C1-C6-alkyl, unsubstituted or substituted C2-C6-alkenyl, unsubstituted or substituted C2-C6-alkynyl or C1-C6-alkoxy, unsubstituted or substituted aryl, halogen, cyano or hydroxy. Efficacy of benzothiazole derivs. in exptl. model of type II diabetes was studied. Oral formulations of benzothiazole compound of formula I is described.				
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	345986-78-9	345986-81-4	345986-84-7		
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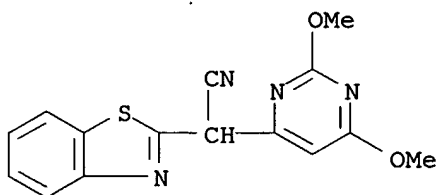
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RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL  
 (Biological study); USES (Uses)

(benzothiazole derivs. for treatment of diabetes)

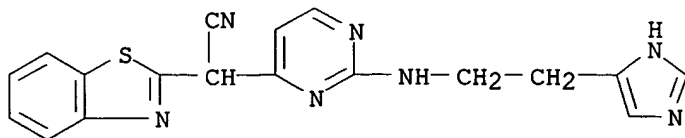
RN 345986-40-5 CAPLUS

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 (CA INDEX NAME)



RN 345986-64-3 CAPLUS

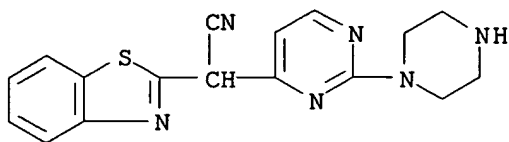
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 4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 345986-66-5 CAPLUS

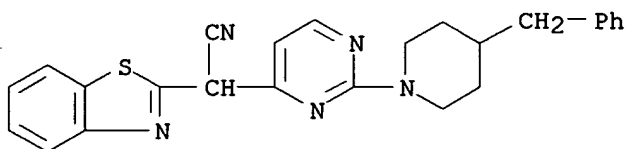
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(1-piperazinyl)-4-pyrimidinyl]-

(9CI) (CA INDEX NAME)



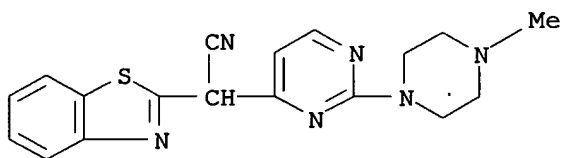
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CN 2-Benzothiazoleacetonitrile, α-[2-[4-(phenylmethyl)-1-piperidinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



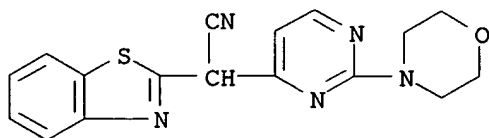
RN 345986-72-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(4-methyl-1-piperazinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



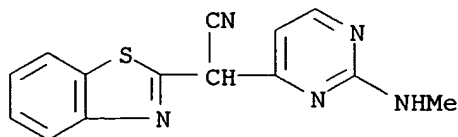
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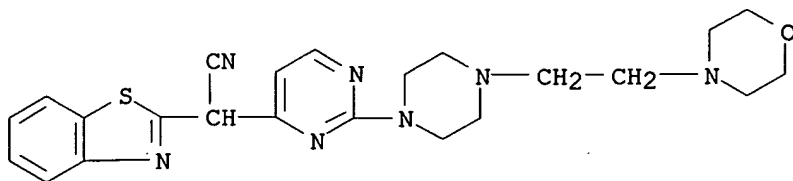


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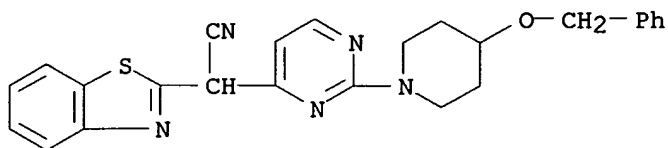
CN 2-Benzothiazoleacetonitrile, α-[2-(methylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



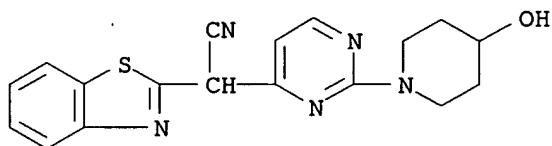
RN 345986-81-4 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[4-[2-(4-morpholinyl)ethyl]-1-piperazinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

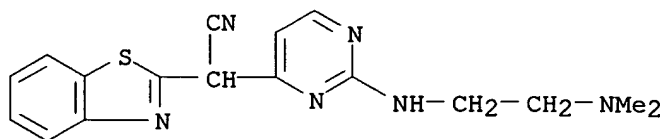
RN 345986-84-7 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[4-(phenylmethoxy)-1-piperidinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345986-86-9 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(4-hydroxy-1-piperidinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

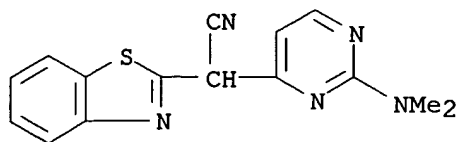
RN 345986-91-6 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(dimethylamino)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345986-94-9 CAPLUS

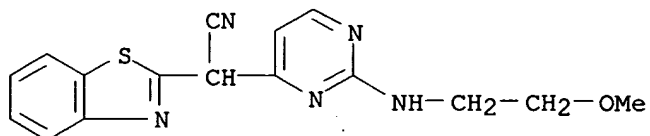
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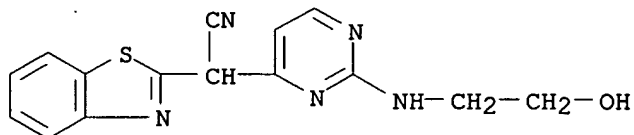
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CN 2-Benzothiazoleacetonitrile, α-[2-[(2-methoxyethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



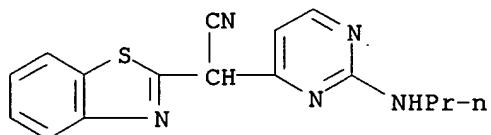
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CN 2-Benzothiazoleacetonitrile, α-[2-[(2-hydroxyethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



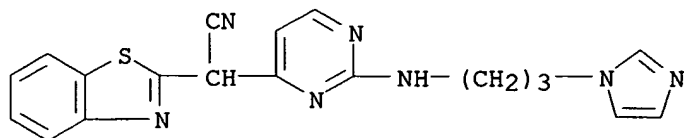
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CN 2-Benzothiazoleacetonitrile, α-[2-(propylamino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 345987-00-0 CAPLUS

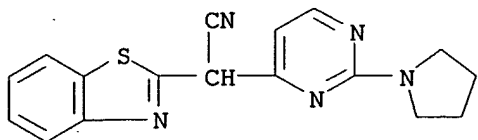
CN 2-Benzothiazoleacetonitrile, α-[2-[(3-(1H-imidazol-1-yl)propyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 345987-02-2 CAPLUS

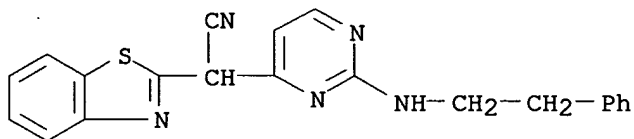
CN 2-Benzothiazoleacetonitrile, α-[2-(1-pyrrolidinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

(9CI) (CA INDEX NAME)



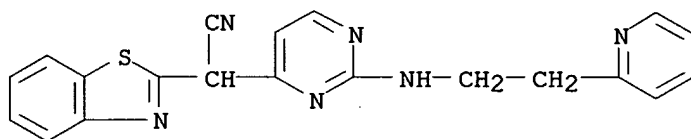
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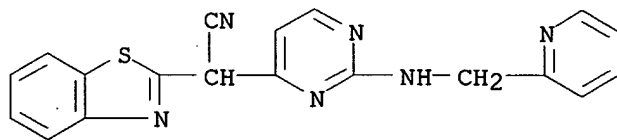
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CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(2-pyridinyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



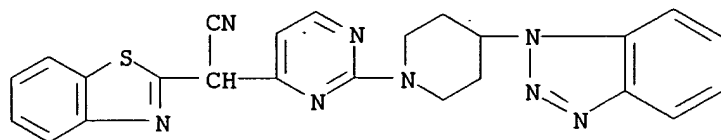
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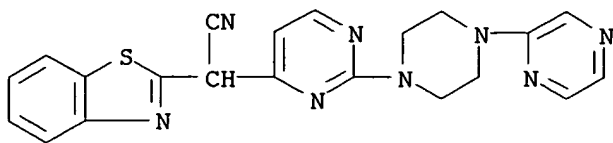


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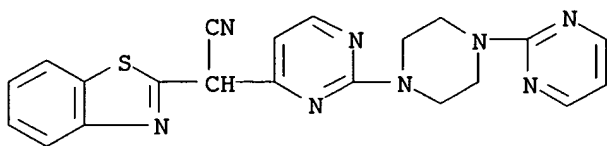
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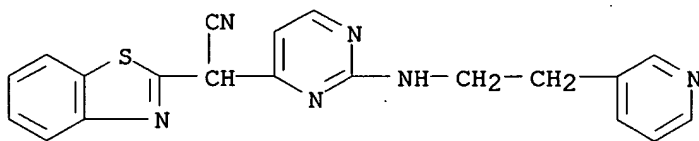
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CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(4-pyrazinyl-1-piperazinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

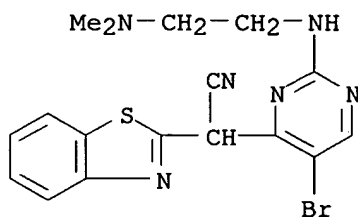
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CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[4-(2-pyrimidinyl)-1-piperazinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345987-15-7 CAPLUS

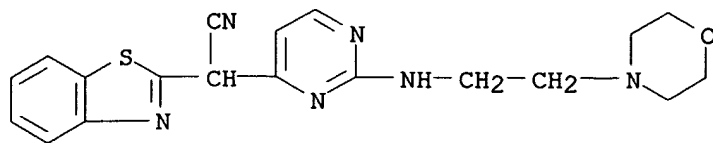
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RN 345987-17-9 CAPLUS

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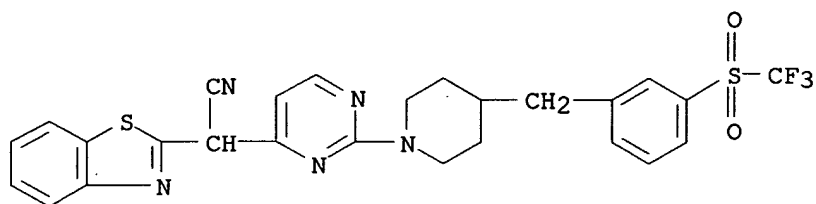
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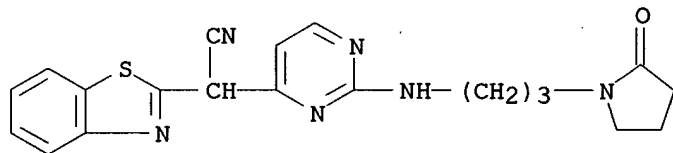
RN 848343-81-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[4-[[3-[(trifluoromethyl)sulfonyl]phenyl]methyl]-1-piperidinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



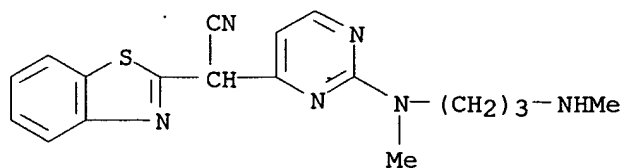
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CN 2-Benzothiazoleacetonitrile, α-[2-[[3-(2-oxo-1-pyrrolidinyl)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



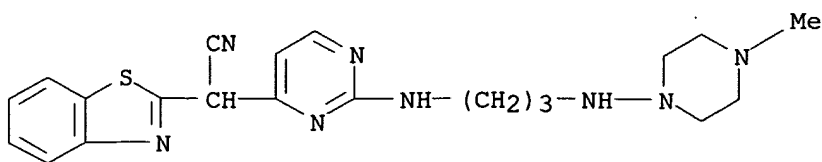
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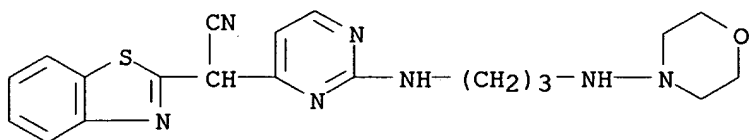
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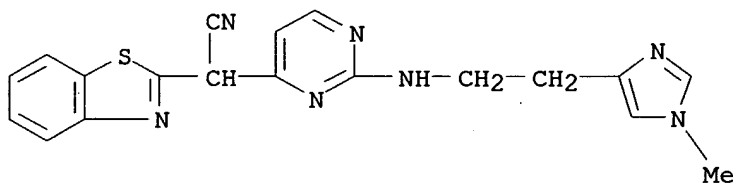
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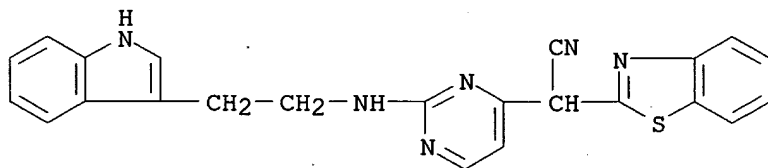
RN 848343-86-2 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(1-methyl-1H-imidazol-4-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



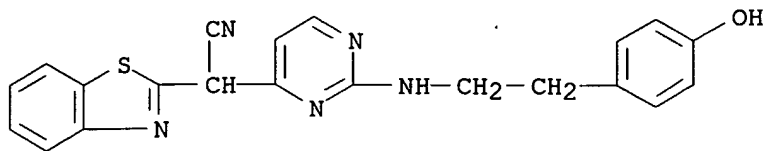
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CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(1H-indol-3-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



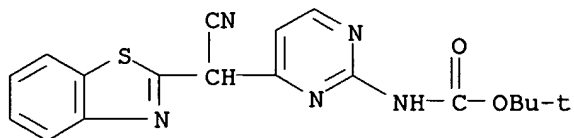
RN 848343-88-4 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



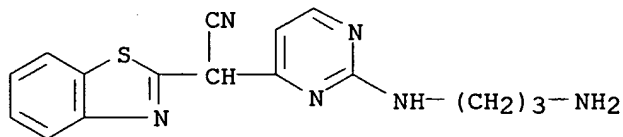
RN 848343-89-5 CAPLUS

CN Carbamic acid, [4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



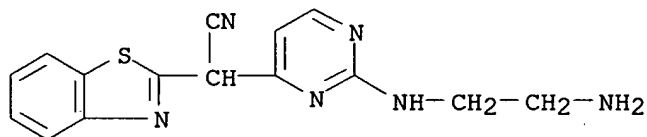
RN 848343-90-8 CAPLUS

CN 2-Benzothiazoleacetone nitrile,  $\alpha$ -[2-[(3-aminopropyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



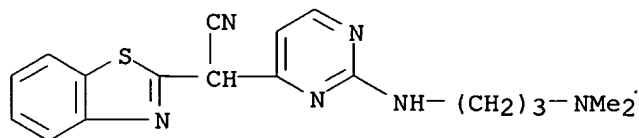
RN 848343-91-9 CAPLUS

CN 2-Benzothiazoleacetone nitrile,  $\alpha$ -[2-[(2-aminoethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 848343-92-0 CAPLUS

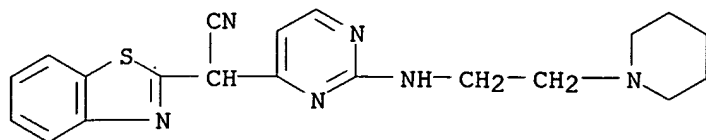
CN 2-Benzothiazoleacetone nitrile,  $\alpha$ -[2-[[3-(dimethylamino)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



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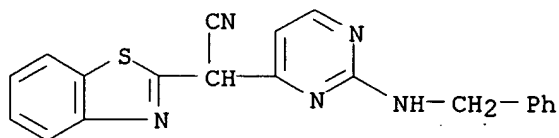
CN 2-Benzothiazoleacetone nitrile,  $\alpha$ -[2-[[2-(1-piperidinyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

pyrimidinyl]- (9CI) (CA INDEX NAME)



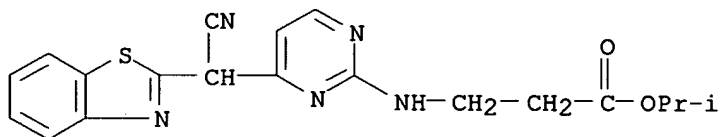
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CN 2-Benzothiazoleacetonitrile, α-[2-[(phenylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



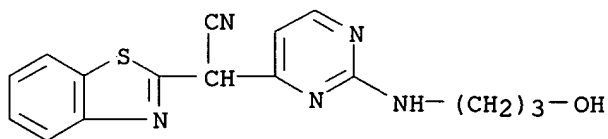
RN 848343-95-3 CAPLUS

CN β-Alanine, N-[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)



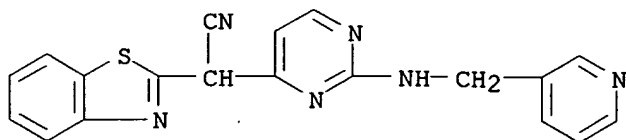
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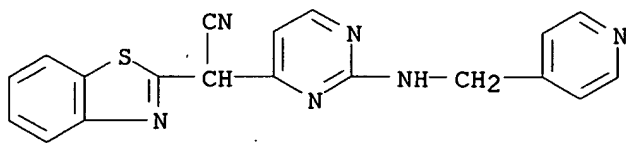


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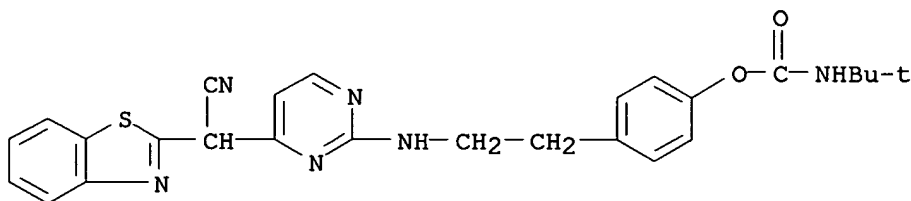


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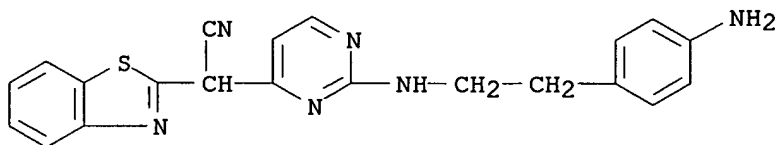
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[(4-pyridinylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848343-99-7 CAPLUS

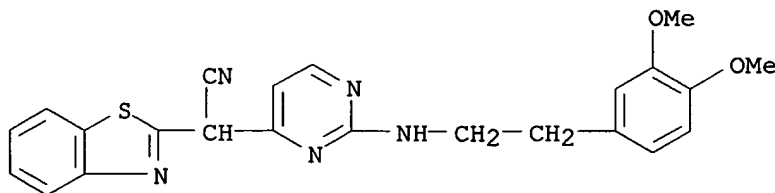
CN Carbamic acid, (1,1-dimethylethyl)-, 4-[2-[[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]amino]ethyl]phenyl ester (9CI) (CA INDEX NAME)



RN 848344-00-3 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(4-aminophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

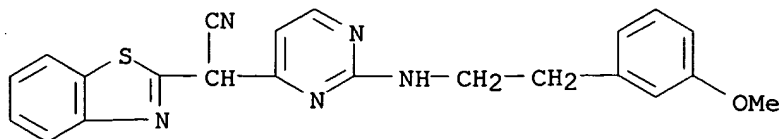
RN 848344-01-4 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-02-5 CAPLUS

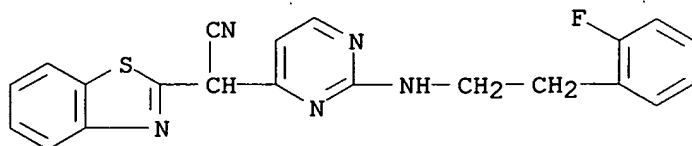
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(3-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)





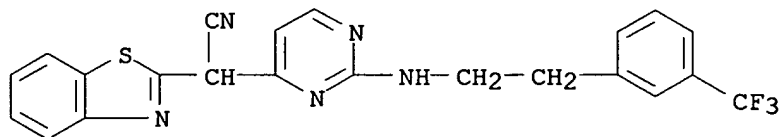
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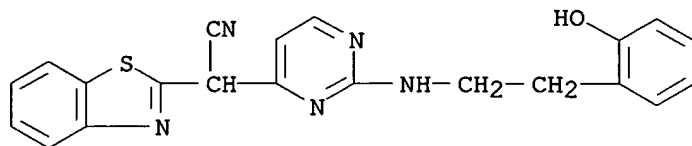
RN 848344-04-7 CAPLUS

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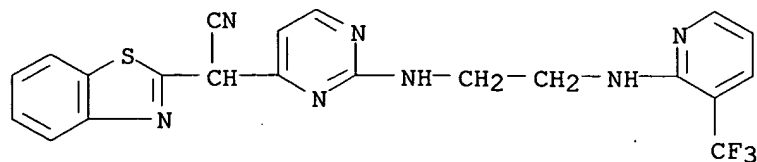
RN 848344-05-8 CAPLUS

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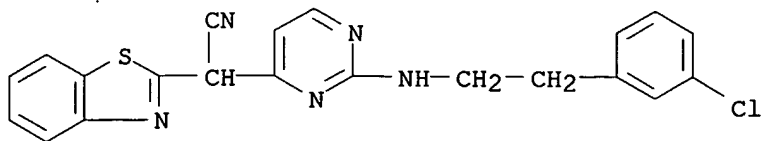
RN 848344-06-9 CAPLUS

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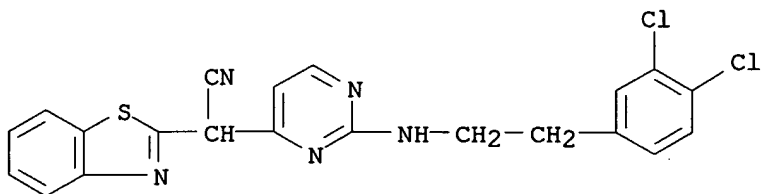
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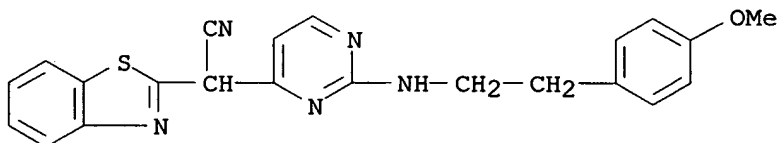
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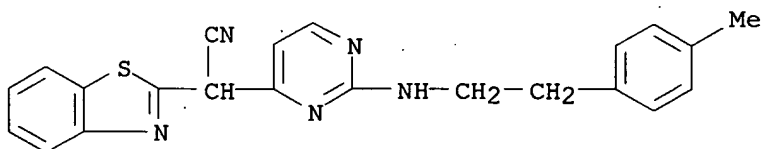
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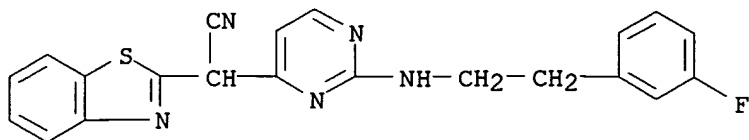
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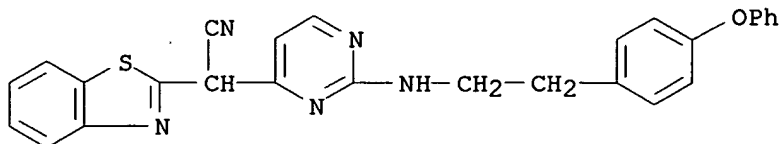
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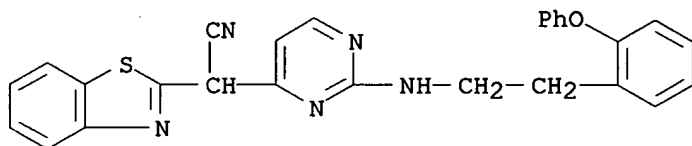
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CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(4-phenoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



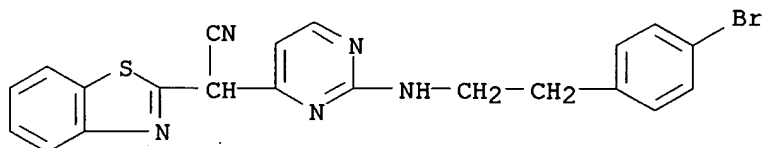
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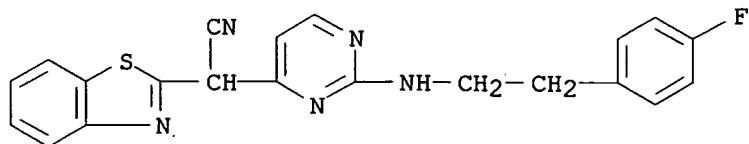
RN 848344-14-9 CAPLUS

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RN 848344-15-0 CAPLUS

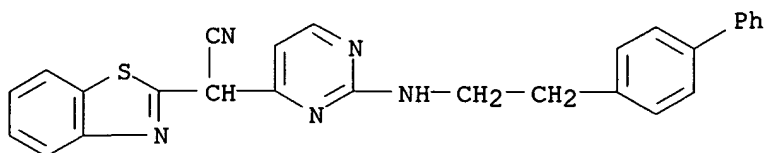
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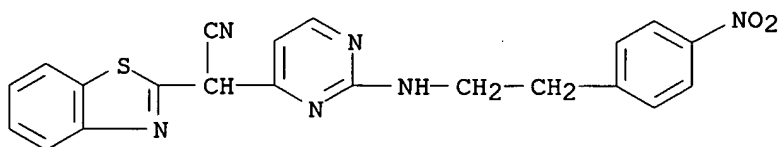
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CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(1,1'-biphenyl)-4-

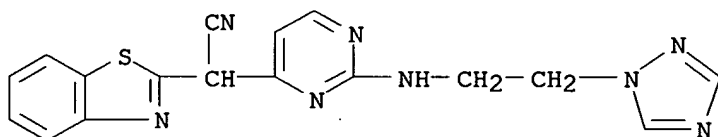
ylethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



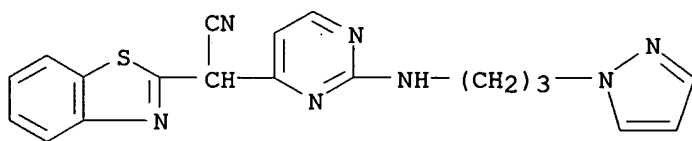
RN 848344-17-2 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(4-nitrophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-18-3 CAPLUS

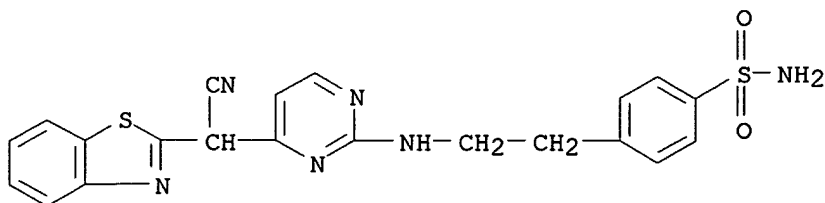
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(1H-1,2,4-triazol-1-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-19-4 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[3-(1H-pyrazol-1-yl)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

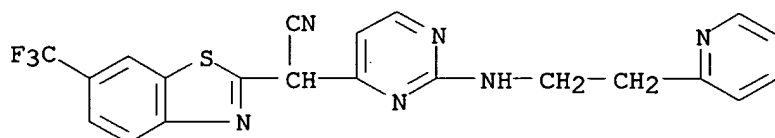
RN 848344-20-7 CAPLUS

CN Benzenesulfonamide, 4-[2-[[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)



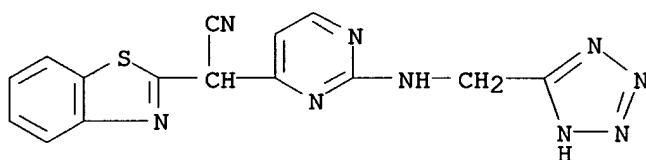
RN 848344-21-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-(2-pyridinyl)ethyl)amino]-4-pyrimidinyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)



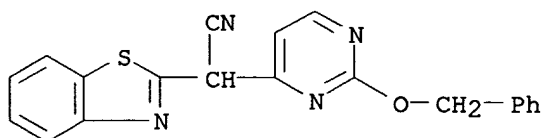
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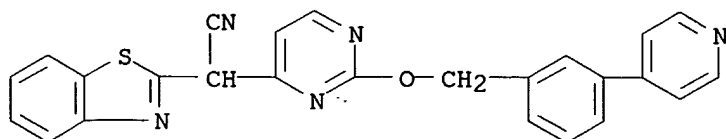
RN 848344-23-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(phenylmethoxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

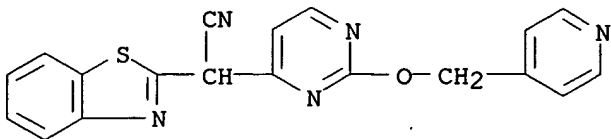


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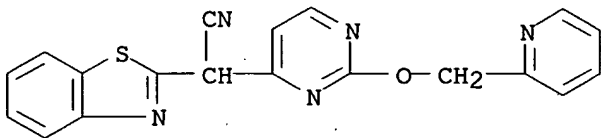
CN 2-Benzothiazoleacetonitrile, α-[2-[(3-(4-pyridinyl)phenyl)methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



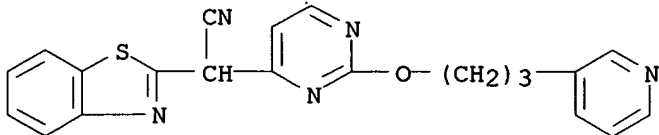
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CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(4-pyridinylmethoxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

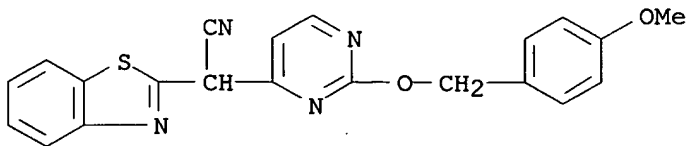
RN 848344-26-3 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(2-pyridinylmethoxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-27-4 CAPLUS

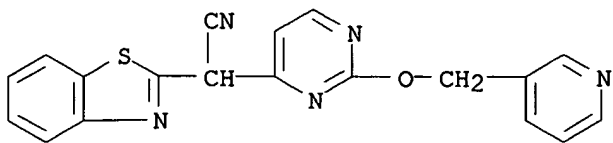
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[3-(3-pyridinyl)propoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-28-5 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[(4-methoxyphenyl)methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

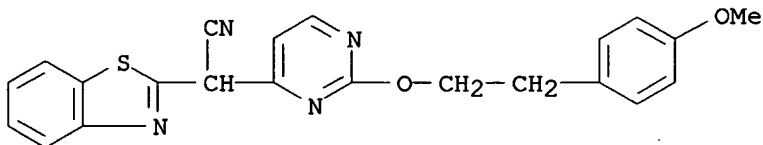
RN 848344-29-6 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(3-pyridinylmethoxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



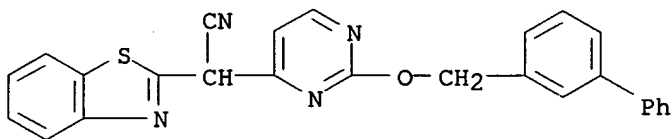
RN 848344-30-9 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[2-(4-methoxyphenyl)ethoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



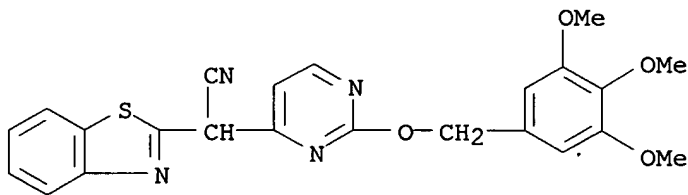
RN 848344-31-0 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-([1,1'-biphenyl]-3-ylmethoxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



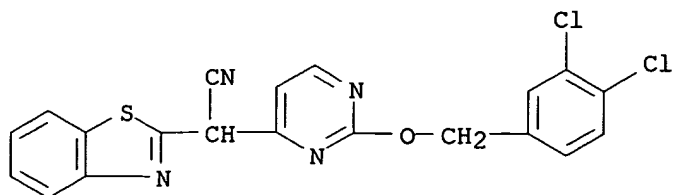
RN 848344-32-1 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[(3,4,5-trimethoxyphenyl)methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



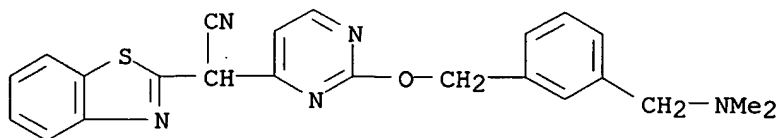
RN 848344-33-2 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[(3,4-dichlorophenyl)methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



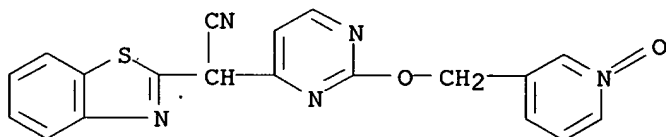
RN 848344-34-3. CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[3-[(dimethylamino)methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



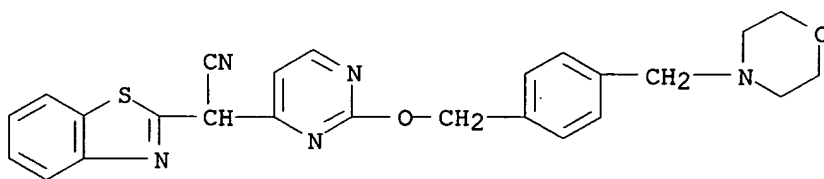
RN 848344-35-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(1-oxido-3-pyridinyl)methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



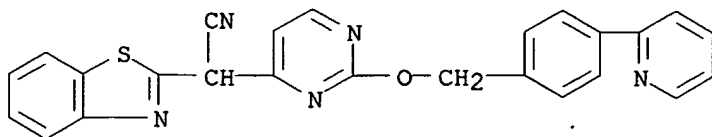
RN 848344-36-5 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(4-morpholinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



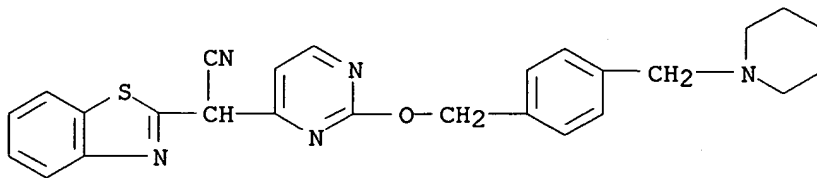
RN 848344-37-6 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(2-pyridinyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

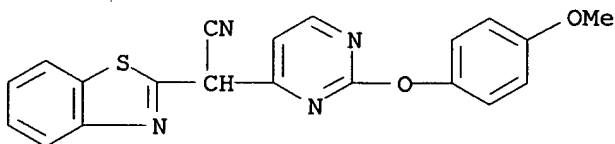




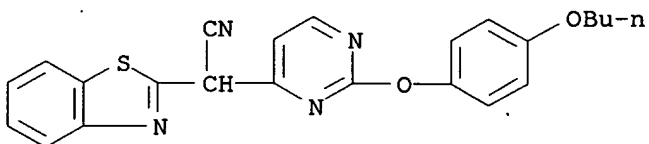
RN 848344-38-7 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[4-(1-piperidinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-39-8 CAPLUS

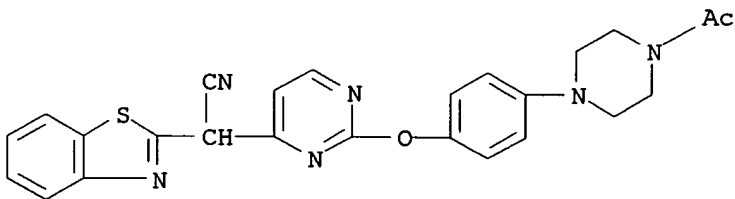
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(4-methoxyphenoxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 848344-40-1 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(4-butoxyphenoxy)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

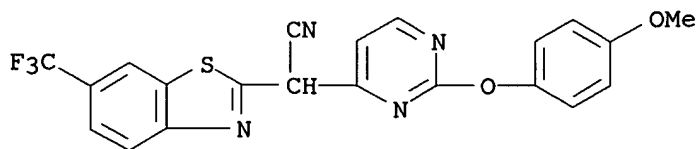
RN 848344-41-2 CAPLUS

CN Piperazine, 1-acetyl-4-[4-[[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]oxy]phenyl]- (9CI) (CA INDEX NAME)



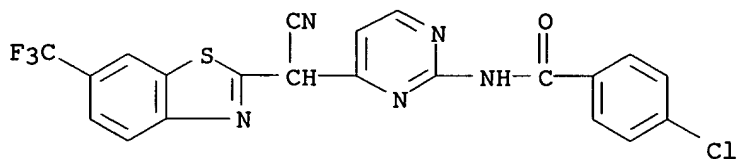
RN 848344-42-3 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(4-methoxyphenoxy)-4-pyrimidinyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)



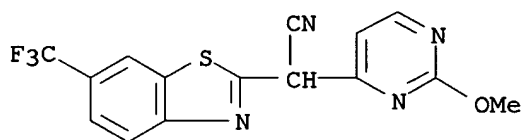
RN 848344-43-4 CAPLUS

CN Benzamide, 4-chloro-N-[4-[cyano[6-(trifluoromethyl)-2-benzothiazolyl]methyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



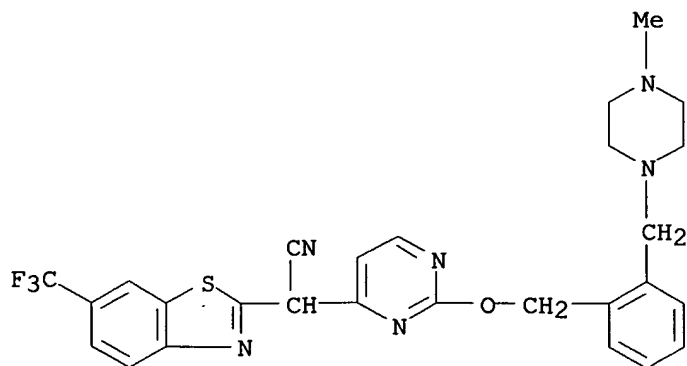
RN 848344-44-5 CAPLUS

CN 2-Benzothiazoleacetone nitrile, alpha-(2-methoxy-4-pyrimidinyl)-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 848344-45-6 CAPLUS

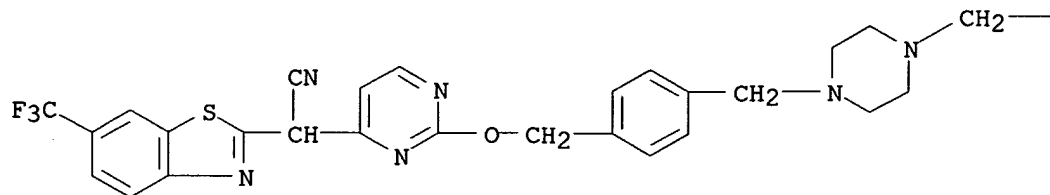
CN 2-Benzothiazoleacetone nitrile, alpha-[2-[[2-[[4-methyl-1-piperazinyl]methyl]phenyl]methoxy]-4-pyrimidinyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 848344-46-7 CAPLUS

CN 2-Benzothiazoleacetone nitrile, alpha-[2-[[4-[[4-(phenylmethyl)-1-piperazinyl]methyl]phenyl]methoxy]-4-pyrimidinyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

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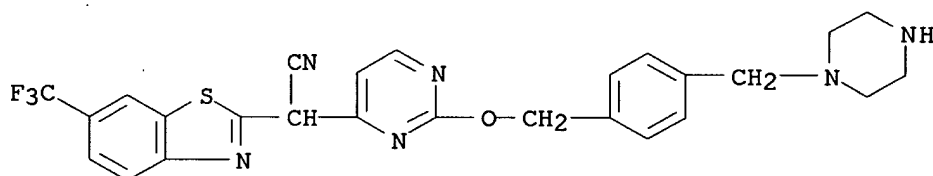


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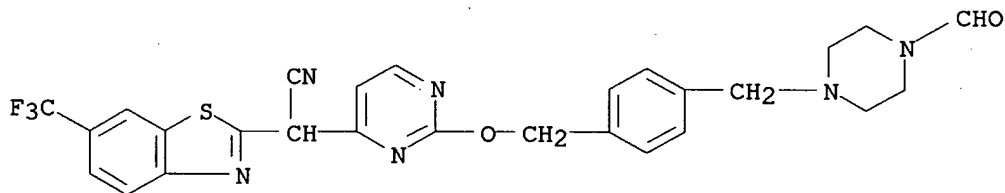
RN 848344-47-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-(1-piperazinylmethyl)phenyl]methoxy]-4-pyrimidinyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)



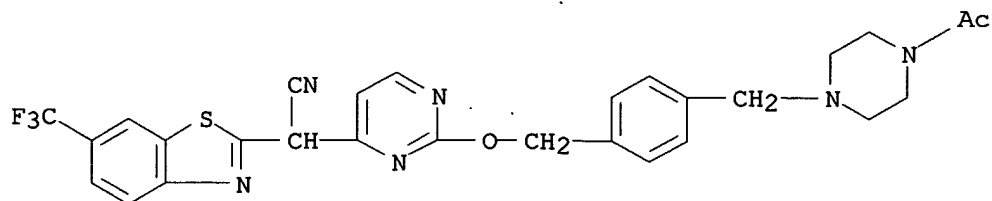
RN 848344-48-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-[(4-formyl-1-piperazinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 848344-49-0 CAPLUS

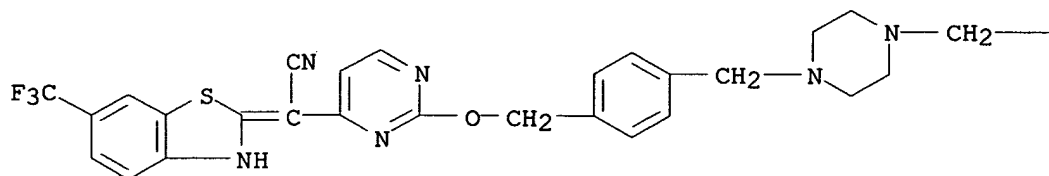
CN Piperazine, 1-acetyl-4-[[4-[[[4-[cyano[6-(trifluoromethyl)-2-benzothiazolyl]methyl]-2-pyrimidinyl]oxy]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



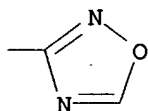
RN 848344-50-3 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-[[4-[[4-(1,2,4-oxadiazol-3-ylmethyl)-1-piperazinyl]methyl]phenyl]methoxy]-α-[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]- (9CI) (CA INDEX NAME)

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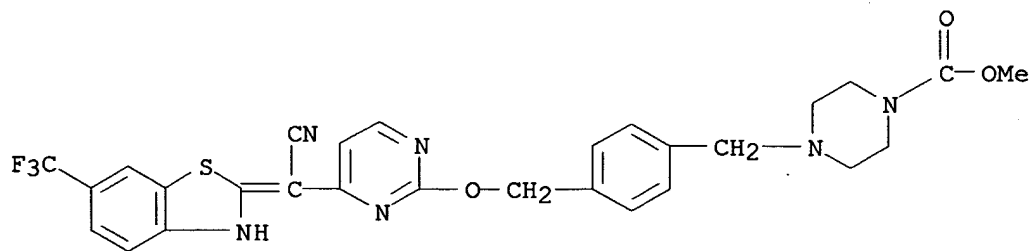


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RN 848344-51-4 CAPLUS

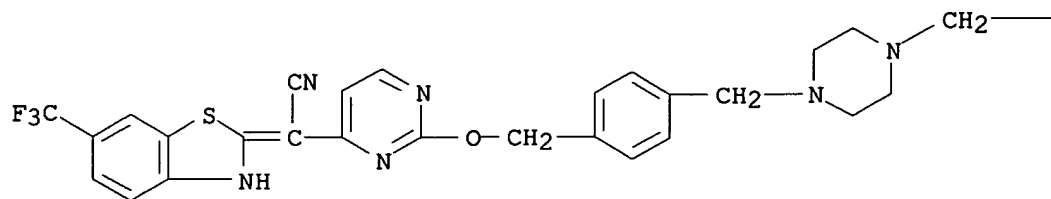
CN 1-Piperazinecarboxylic acid, 4-[[4-[[[4-[cyano[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]methyl]-2-pyrimidinyl]oxy]methyl]phenyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)



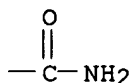
RN 848344-52-5 CAPLUS

CN 1-Piperazineacetamide, 4-[[4-[[[4-[cyano[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]methyl]-2-pyrimidinyl]oxy]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

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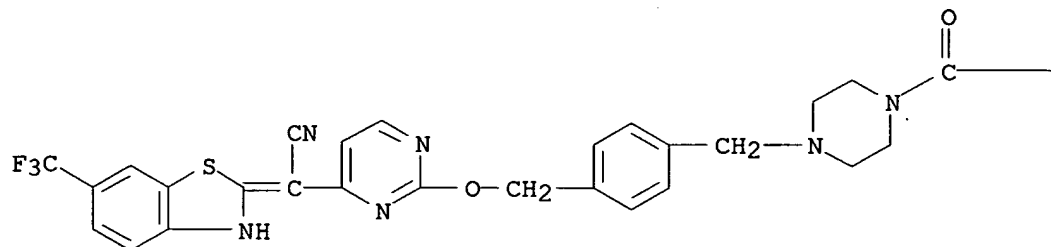
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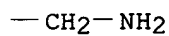
RN 848344-53-6 CAPLUS

CN Piperazine, 1-(aminoacetyl)-4-[[4-[[[4-[cyano[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]methyl]-2-pyrimidinyl]oxy]methyl]phenyl]methyl]- (9CI)  
(CA INDEX NAME)

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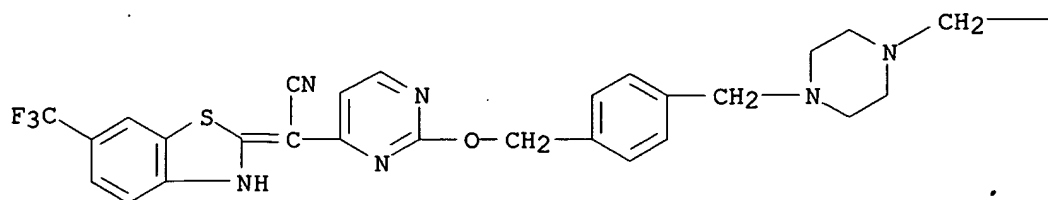
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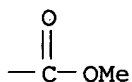
RN 848344-54-7 CAPLUS

CN 1-Piperazineacetic acid, 4-[[4-[[[4-[cyano[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]methyl]-2-pyrimidinyl]oxy]methyl]phenyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

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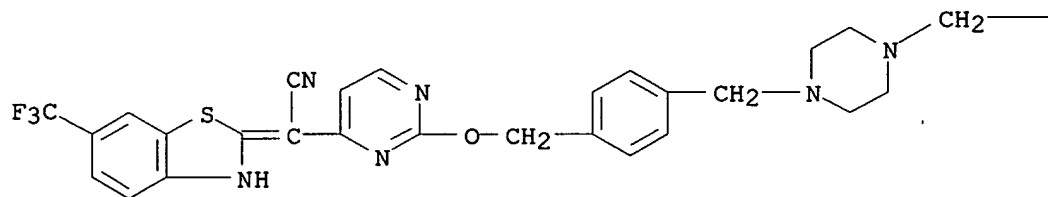
PAGE 1-B



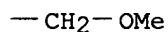
RN 848344-55-8 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-[[4-[[4-(2-methoxyethyl)-1-piperazinyl]methyl]phenyl]methoxy]- $\alpha$ -[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]- (9CI) (CA INDEX NAME)

PAGE 1-A

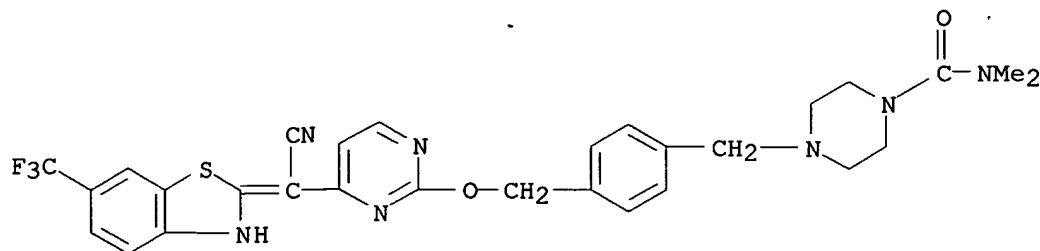


PAGE 1-B



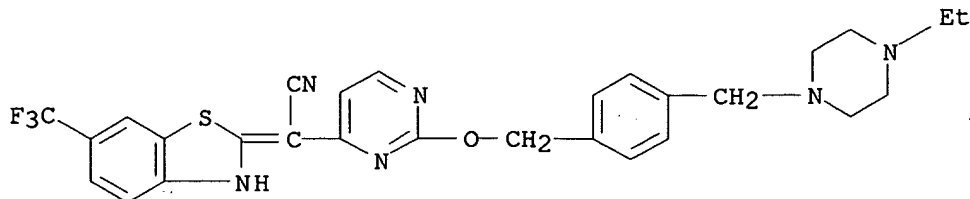
RN 848344-56-9 CAPLUS

CN 1-Piperazinecarboxamide, 4-[[4-[[[4-[cyano[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]methyl]-2-pyrimidinyl]oxy]methyl]phenyl]methyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



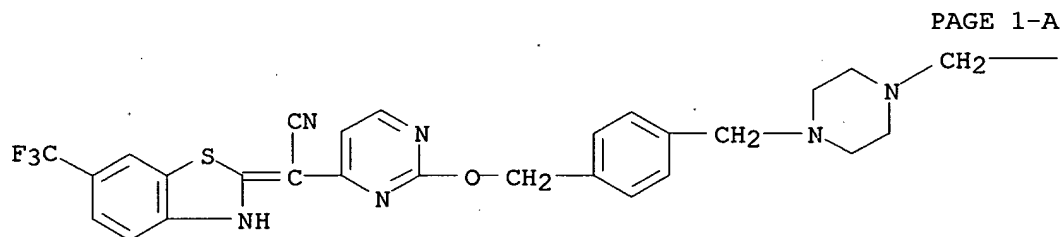
RN 848344-57-0 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-[[4-[(4-ethyl-1-piperazinyl)methyl]phenyl]methoxy]- $\alpha$ -[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]- (9CI) (CA INDEX NAME)



RN 848344-58-1 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-[[4-[[4-(2-hydroxyethyl)-1-piperazinyl]methyl]phenyl]methoxy]- $\alpha$ -[6-(trifluoromethyl)-2(3H)-benzothiazolylidene]- (9CI) (CA INDEX NAME)



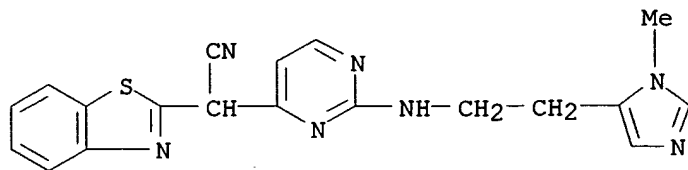
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PAGE 1-B

—CH<sub>2</sub>—OH

RN 848344-70-7 CAPLUS

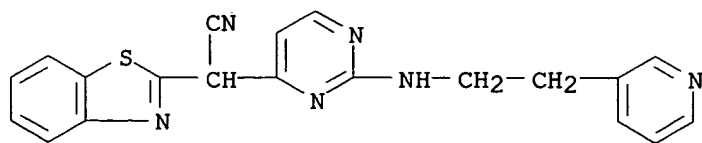
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(1-methyl-1H-imidazol-5-yl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RE.CNT 3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

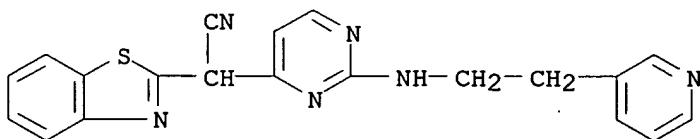
L4 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2005:233187 CAPLUS  
 DN 142:259314  
 TI Control of death receptor and mitochondrial-dependent apoptosis by c-Jun  
 N-terminal kinase in hippocampal CA1 neurones following global transient  
 ischemia  
 AU Carboni, Sonia; Antonsson, Bruno; Gaillard, Pascale; Gotteland,  
 Jean-Pierre; Gillon, Jean-Yves; Vitte, Pierre-Alain  
 CS Department of Pharmacology, Sero Pharmaceutical Research Institute,  
 Geneva, 1228, Switz.  
 SO Journal of Neurochemistry (2005), 92(5), 1054-1060  
 CODEN: JONRA9; ISSN: 0022-3042  
 PB Blackwell Publishing Ltd.  
 DT Journal  
 LA English  
 AB C-Jun N-terminal kinase (JNK), a member of the mitogen-activated protein  
 kinase family, is activated in response to a number of extracellular stimuli,  
 including inflammatory cytokines, UV irradiation and ischemia. A large body  
 of evidence supports a role for JNK signaling in stress-induced apoptosis.  
 It has been hypothesized that JNK may contribute to the apoptotic response  
 by regulating the intrinsic cell death pathway involving the mitochondria.  
 Here, we examined the role of the JNK signaling pathway in hippocampal CA1  
 apoptotic neurons following transient ischemia in gerbils. We showed  
 early activation of death receptor-dependent apoptosis (caspase-8  
 activation 2 days after ischemia) and a biphasic activation of caspase-3  
 and caspase-9 after ischemia. Activation of the mitochondrial pathway, as  
 measured by cytochrome c release, appeared as a late event (5-7 days after  
 ischemia). AS601245, a novel JNK inhibitor, antagonized activation of  
 both pathways and significantly protected CA1 neurons from cell death.  
 Our results suggest a key role of JNK in the control of death receptor and  
 mitochondrial-dependent apoptosis after transient ischemia.  
 IT 345987-15-7, AS601245  
 RL: BUU (Biological use, unclassified); PAC (Pharmacological activity);  
 THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (AS601245, JNK inhibitor, antagonized activation of apoptotic and  
 significantly protected CA1 neurons from cell death.)  
 RN 345987-15-7 CAPLUS  
 CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(3-pyridinyl)ethyl]amino]-4-  
 pyrimidinyl]- (9CI) (CA INDEX NAME)



RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

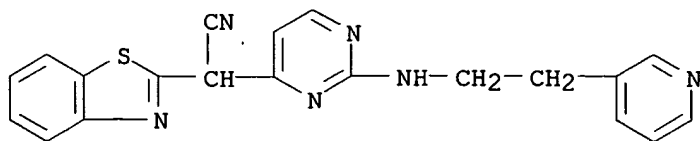


L4 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2005:146539 CAPLUS  
 DN 142:328799  
 TI Targeting the JNK signaling pathway for stroke and Parkinson's diseases therapy  
 AU Kuan, Chia-Yi; Burke, Robert E.  
 CS Division of Developmental Biology, Cincinnati Children's Hospital Research Foundation, Cincinnati, OH, 45229, USA  
 SO Current Drug Targets: CNS & Neurological Disorders (2005), 4(1), 63-67  
 CODEN: CDTCCC; ISSN: 1568-007X  
 PB Bentham Science Publishers Ltd.  
 DT Journal; General Review  
 LA English  
 AB A review. The c-Jun NH2-terminal Kinase (JNK) signaling pathway is frequently induced by cellular stress and correlated with neuronal death. This unique property makes JNK signaling a promising target for developing pharmacol. intervention. Among several neurol. disorders, JNK signaling is particularly implicated in ischemic stroke and Parkinson's disease. The inhibitors of the JNK signaling pathway include upstream kinase inhibitors (for example, CEP-1347), small chemical inhibitors of JNK (SP600125 and AS601245), and peptide inhibitors of the interaction between JNK and its substrates (D-JNKI and I-JIP). The mechanisms by which JNK signaling induces apoptosis and evidence of cytoprotective effects of these JNK inhibitors are summarized in the present review.  
 IT 345987-15-7, AS601245  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (targeting the JNK signaling pathway for stroke and Parkinson's diseases therapy)  
 RN 345987-15-7 CAPLUS  
 CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(3-pyridinyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

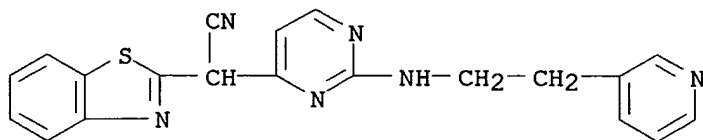
L4 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2004:638580 CAPLUS  
 DN 141:325444  
 TI Inhibition of c-jun N-terminal kinase decreases cardiomyocyte apoptosis and infarct size after myocardial ischemia and reperfusion in anaesthetized rats  
 AU Ferrandi, Chiara; Ballerio, Rossana; Gaillard, Pascale; Giachetti, Claudio; Carboni, Sonia; Vitte, Pierre-Alain; Gotteland, Jean-Pierre; Cirillo, Rocco  
 CS Istituto di Ricerche Biomediche "A. Marxer", LCG-RBM/Serono Discovery, Colletterto Giacosa, I-10010, Italy  
 SO British Journal of Pharmacology (2004), 142(6), 953-960  
 CODEN: BJPCBM; ISSN: 0007-1188  
 PB Nature Publishing Group  
 DT Journal  
 LA English  
 AB 1 Myocardial ischemia/reperfusion is associated with inflammation, apoptosis and necrosis. During this process, c-jun N-terminal kinase is activated in cardiac myocytes resulting in apoptosis. 2 This study investigates the effects of AS601245, a nonpeptide ATP competitive JNK inhibitor, on infarct size caused by myocardial ischemia/reperfusion in anesthetized rats. The left descending coronary artery of anesthetized rats was occluded for 30 min and then reperfused for 3 h. AS601245 was administered 5 min before the end of the ischemia period as an i.v. bolus (1.5, 4.5 or 15 mg kg<sup>-1</sup> i.v.) followed by continuous i.v. infusion (18, 55 and 183 µg kg<sup>-1</sup> min<sup>-1</sup>, resp.) during reperfusion. Controls received saline only. 3-Aminobenzamide, a poly(ADP-ribose) polymerase inhibitor, was used as reference compound at 10 mg kg<sup>-1</sup> i.v. bolus plus 0.17 mg kg<sup>-1</sup> min<sup>-1</sup> continuous infusion. 3 AS601245 significantly reduced infarct size at 4.5 mg kg<sup>-1</sup> (-44%) and 15 mg kg<sup>-1</sup> i.v. (-40.3%) similarly to 3-aminobenzamide (-44.2%). This protective effect was obtained without affecting hemodynamics or reducing ST-segment displacement. 4 The beneficial effects on infarct size correlated well with the reduction of c-jun phosphorylation (-85%; vs. control) and of TUNEL-pos. cells (-82.1%) in post-ischemic cardiomyocytes. No change in the phosphorylation state of p38 MAPK and ERK in post-ischemic heart was observed in the presence of AS601245 in comparison to the vehicle-treated group. 5 These results demonstrate that blocking the JNK pathway may represent a novel therapeutic approach for treating myocardial ischemia/reperfusion-induced cardiomyocyte death.  
 IT 345987-15-7, AS 601245  
 RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (inhibition of c-jun N-terminal kinase with AS601245 decreases cardiomyocyte apoptosis and infarct size after myocardial ischemia and reperfusion in anesthetized rats)  
 RN 345987-15-7 CAPLUS  
 CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3-pyridinyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



10/511,438

RE.CNT 23      THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2004:547002 CAPLUS  
 DN 141:218787  
 TI AS601245 (1,3-benzothiazol-2-yl (2-([2-(3-pyridinyl) ethyl] amino)-4-pyrimidinyl) acetonitrile): A c-Jun NH2-terminal protein kinase inhibitor with neuroprotective properties  
 AU Carboni, Sonia; Hiver, Agnes; Szyndralewicz, Cedric; Gaillard, Pascale; Gotteland, Jean-Pierre; Vitte, Pierre-Alain  
 CS Department of Pharmacology, Sero Pharmaceutical Research Institute, Geneva, Switz.  
 SO Journal of Pharmacology and Experimental Therapeutics (2004), 310(1), 25-32  
 CODEN: JPETAB; ISSN: 0022-3565  
 PB American Society for Pharmacology and Experimental Therapeutics  
 DT Journal  
 LA English  
 AB Recent evidence suggests that activation of the c-Jun NH2-terminal protein kinase (JNK) signal transduction pathway may play a role in ischemia-induced cell death. Thus, preventing the activation of JNK, or c-Jun phosphorylation could be neuroprotective. In the current study, we report that a small mol., AS601245 (1,3-benzothiazol-2-yl-(2-([2-(3-pyridinyl)ethyl]amino)-4-pyrimidinyl) acetonitrile), which has been shown to inhibit the JNK signaling pathway, promotes cell survival after cerebral ischemia. In vivo, AS601245 (40, 60, and 80 mg/kg) administered i.p. provided significant protection against the delayed loss of hippocampal CA1 neurons in a gerbil model of transient global ischemia. This effect is mediated by JNK inhibition and therefore by c-Jun expression and phosphorylation. A significant neuroprotective effect of AS601245 administered either by i.p. injection (6, 18, and 60 mg/kg) or as i.v. bolus (1 mg/kg) followed by an i.v. infusion (0.6 mg/kg/h) was also observed in rats after focal cerebral ischemia. These data suggest that the use of JNK inhibitors such as AS601245 may be a relevant strategy in the therapy of ischemic insults.  
 IT 345987-15-7, AS 601245  
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (JNK inhibitor AS601245 with neuroprotective properties)  
 RN 345987-15-7 CAPLUS  
 CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-([2-(3-pyridinyl)ethyl]amino)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2003:875284 CAPLUS

DN 139:364962

TI Preparation of piperazine benzothiazoles as agents for the treatment of cerebral ischemic disorders or CNS disorders

IN Gaillard, Pascale; Gotteland, Jean-pierre; Vitte, Pierre-alain

PA Applied Research Systems Ars Holding N.V., Neth. Antilles

SO PCT Int. Appl., 46 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003091249	A1	20031106	WO 2003-EP4323	20030425
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2481763	AA	20031106	CA 2003-2481763	20030425
	AU 2003233067	A1	20031110	AU 2003-233067	20030425
	EP 1501828	A1	20050202	EP 2003-727365	20030425
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	CN 1662528	A	20050831	CN 2003-814493	20030425
	JP 2006504631	T2	20060209	JP 2003-587807	20030425
	ZA 2004008023	A	20051005	ZA 2004-8023	20041005
	US 2005261304	A1	20051124	US 2005-511438	20050610
PRAI	EP 2002-100417	A	20020425		
	WO 2003-EP4323	W	20030425		

OS MARPAT 139:364962

AB The title compds. [I; R = H, alkyl, heteroaryl, etc.; R1 = H, halo, CN, etc.; n = 0-3] and their salts that are inhibitors of JNK kinases, in particular of JNK2 and JNK3, and may therefore be used in the treatment and/or prophylaxis of cerebral ischemic disorders or CNS disorders, were prepared and formulated. Thus, treating alc. II with NaH in DMA followed by addition of the benzothiazole III (preps. of reactants given) afforded I [R = Me; R1 = H; n = 1]. The tested compds. I display IC50 of < 10  $\mu$ M with regard to JNK3.

IT 622381-38-8P 622381-39-9P 622381-40-2P

622381-41-3P 622381-42-4P 622381-43-5P

622381-44-6P 622381-45-7P 622381-46-8P

622381-47-9P 622381-48-0P 622381-49-1P

622381-50-4P 622381-51-5P 622381-52-6P

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622381-56-0P 622381-57-1P 622381-58-2P

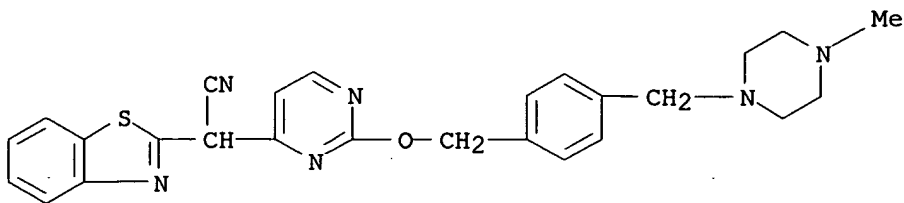
622381-59-3P 622381-60-6P 622381-61-7P

622381-62-8P 622381-63-9P 622381-64-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of piperazine benzothiazoles as inhibitors of JNK kinases)

RN 622381-38-8 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[4-[(4-methyl-1-piperazinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

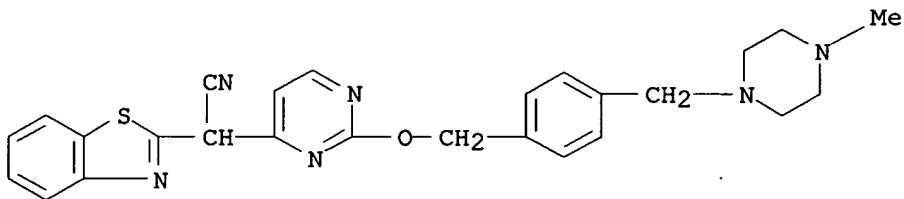
RN 622381-39-9 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[4-[(4-methyl-1-piperazinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]-, trimethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 622381-38-8

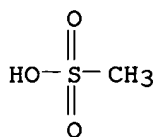
CMF C26 H26 N6 O S



CM 2

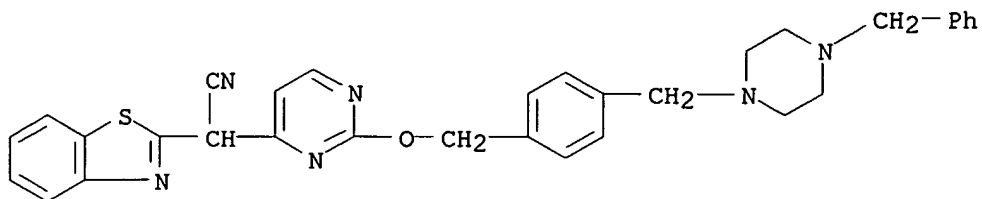
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CMF C H4 O3 S



RN 622381-40-2 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[4-[(4-(phenylmethyl)-1-piperazinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



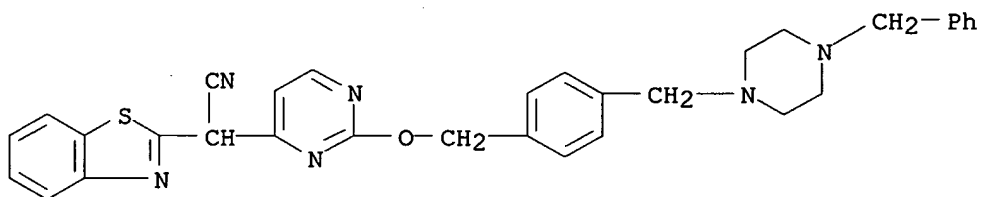
RN 622381-41-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-[[4-(phenylmethyl)-1-piperazinyl]methyl]phenyl]methoxy]-4-pyrimidinyl]-, dimethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 622381-40-2

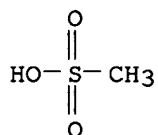
CMF C32 H30 N6 O S



CM 2

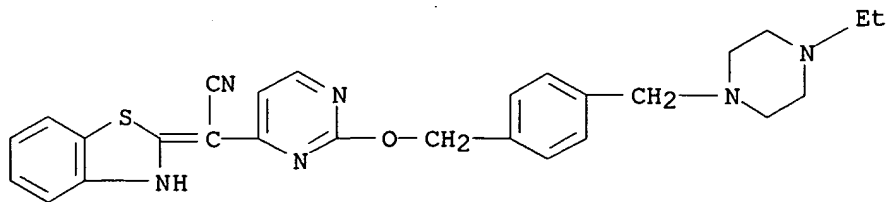
CRN 75-75-2

CMF C H4 O3 S

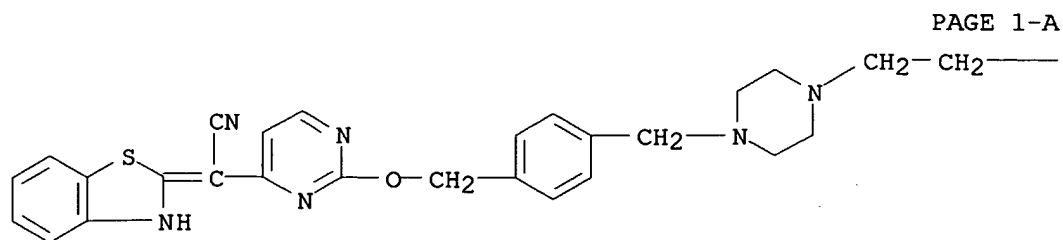


RN 622381-42-4 CAPLUS

CN 4-Pyrimidineacetonitrile, α-2(3H)-benzothiazolylidene-2-[[4-[(4-ethyl-1-piperazinyl)methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)



RN 622381-43-5 CAPLUS  
 CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[4-[[4-(2-methoxyethyl)-1-piperazinyl]methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)



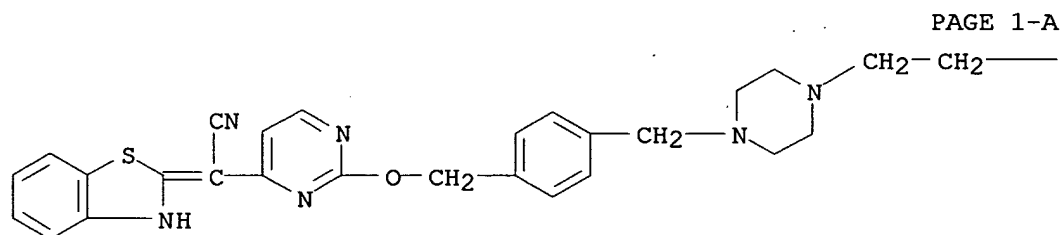
PAGE 1-B

— OMe

RN 622381-44-6 CAPLUS  
 CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[4-[[4-(2-methoxyethyl)-1-piperazinyl]methyl]phenyl]methoxy]-, tris(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 622381-43-5  
 CMF C28 H30 N6 O2 S



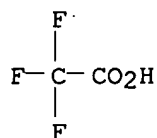
PAGE 1-B

— OMe

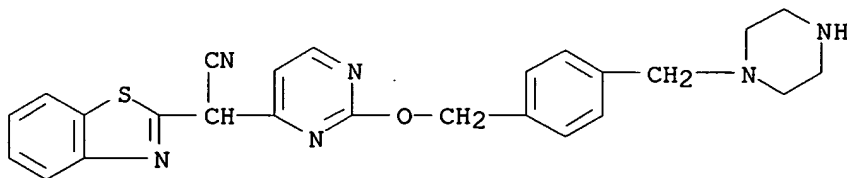
CM 2

CRN 76-05-1  
 CMF C2 H F3 O2





RN 622381-45-7 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[4-(1-piperazinylmethyl)phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

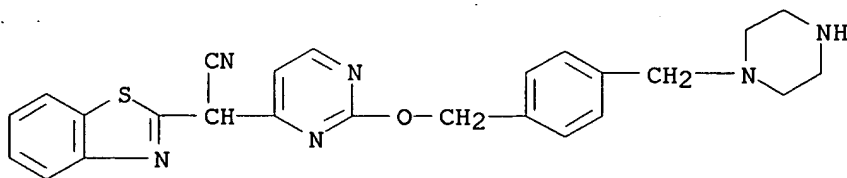
RN 622381-46-8 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[4-(1-piperazinylmethyl)phenyl]methoxy]-4-pyrimidinyl]-, tris(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 622381-45-7

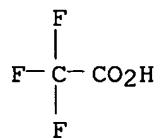
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CM 2

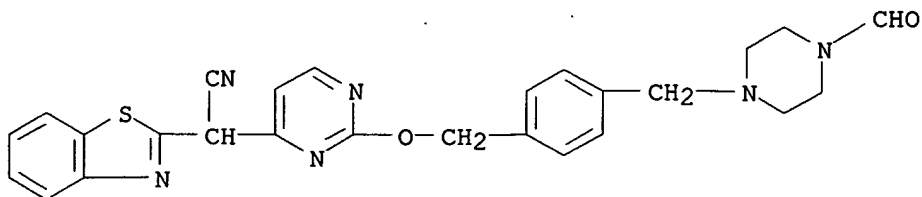
CRN 76-05-1

CMF C2 H F3 O2



RN 622381-47-9 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[4-[(4-formyl-1-piperazinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



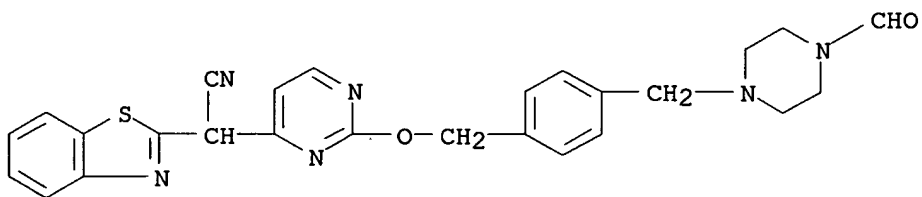
RN 622381-48-0 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[4-[(4-formyl-1-piperazinyl)methyl]phenyl]methoxy]-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 622381-47-9

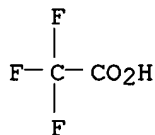
CMF C26 H24 N6 O2 S



CM 2

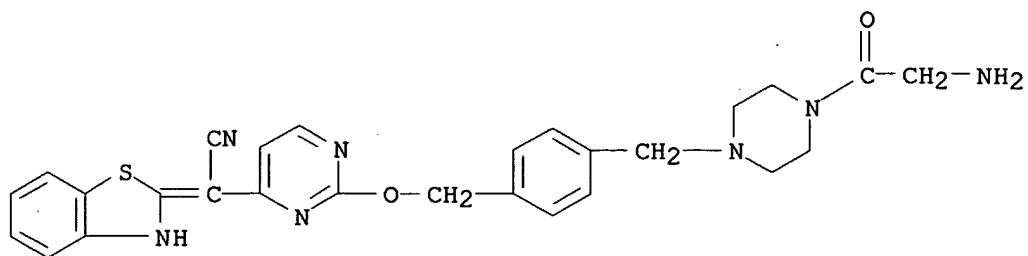
CRN 76-05-1

CMF C2 H F3 O2



RN 622381-49-1 CAPLUS

CN Piperazine, 1-(aminoacetyl)-4-[[4-[[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



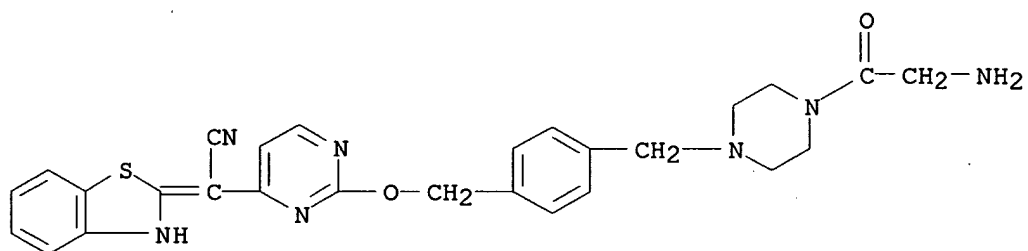
RN 622381-50-4 CAPLUS

CN Piperazine, 1-(aminoacetyl)-4-[[4-[[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl]-, dimethanesulfonate tris(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 622381-49-1

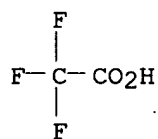
CMF C27 H27 N7 O2 S



CM 2

CRN 76-05-1

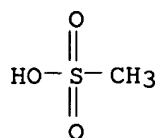
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CM 3

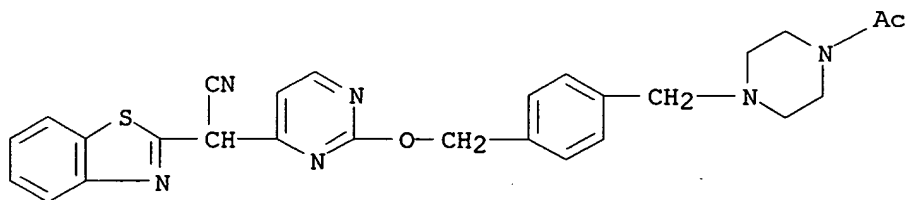
CRN 75-75-2

CMF C H4 O3 S



RN 622381-51-5 CAPLUS

CN Piperazine, 1-acetyl-4-[[4-[[[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl]- (9CI) (CA INDEX NAME)



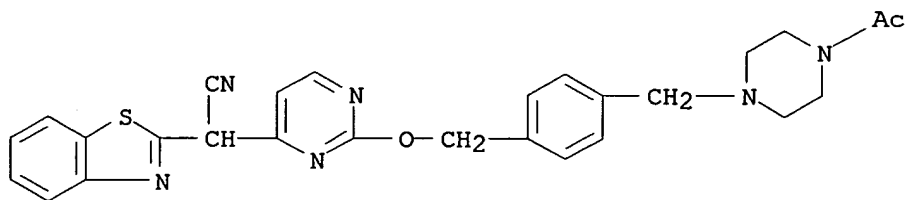
RN 622381-52-6 CAPLUS

CN Piperazine, 1-acetyl-4-[[4-[[[4-(2-benzothiazolylcyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 622381-51-5

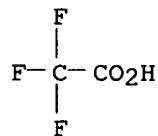
CMF C27 H26 N6 O2 S



CM 2

CRN 76-05-1

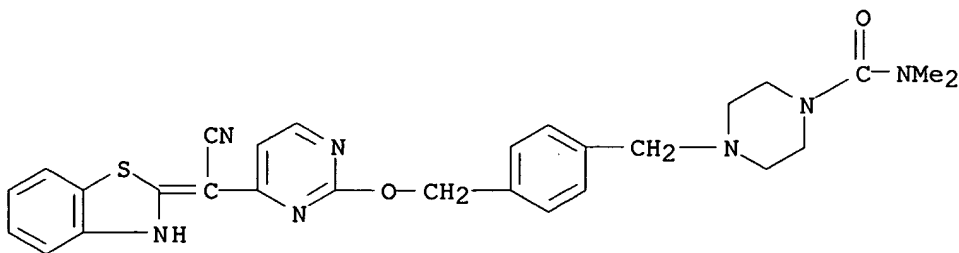
CMF C2 H F3 O2



RN 622381-53-7 CAPLUS

CN 1-Piperazinecarboxamide, 4-[[4-[[[4-(2(3H)-benzothiazolylidenecyanomethyl)-

2-pyrimidinyl]oxy)methyl]phenyl)methyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



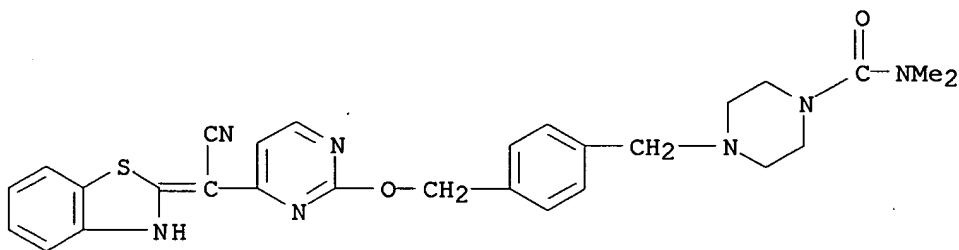
RN 622381-54-8 CAPLUS

CN 1-Piperazinecarboxamide, 4-[[[4-[(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy)methyl]phenyl)methyl]-N,N-dimethyl-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 622381-53-7

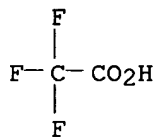
CMF C28 H29 N7 O2 S



CM 2

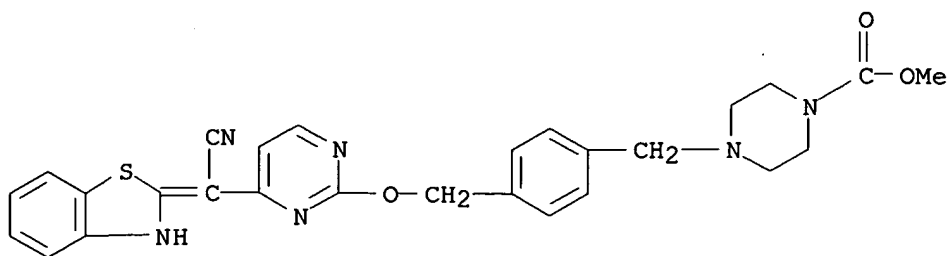
CRN 76-05-1

CMF C2 H F3 O2



RN 622381-55-9 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[4-[(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy)methyl]phenyl)methyl]-, methyl ester (9CI) (CA INDEX NAME)



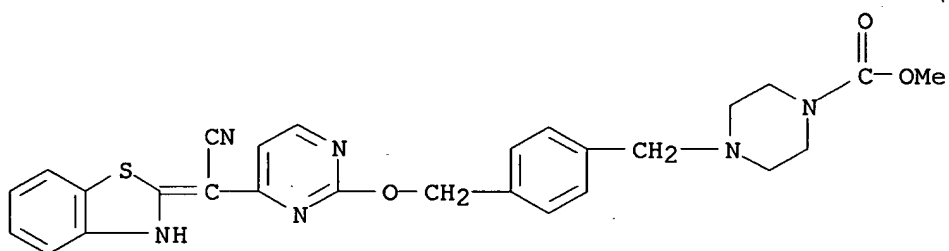
RN 622381-56-0 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[[4-[[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy)methyl]phenyl]methyl]-, methyl ester, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 622381-55-9

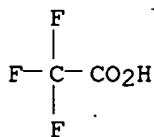
CMF C27 H26 N6 O3 S



CM 2

CRN 76-05-1

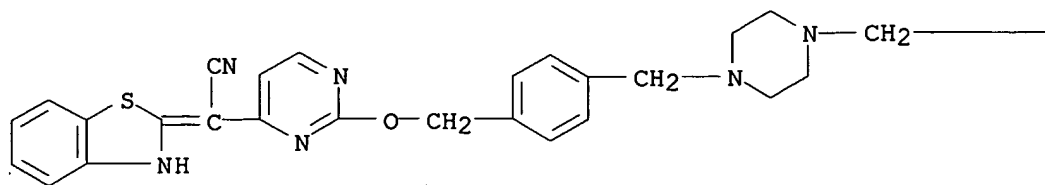
CMF C2 H F3 O2



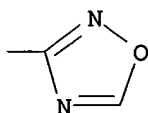
RN 622381-57-1 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[[4-[[[4-(1,2,4-oxadiazol-3-ylmethyl)-1-piperazinyl]methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

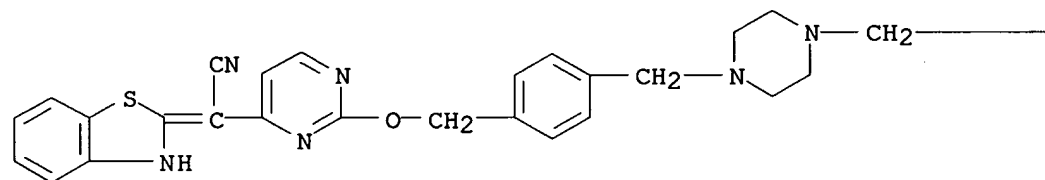


RN 622381-58-2 CAPLUS  
 CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[4-[[4-(1,2,4-oxadiazol-3-ylmethyl)-1-piperazinyl]methyl]phenyl]methoxy]-, tris(trifluoroacetate) (9CI) (CA INDEX NAME)

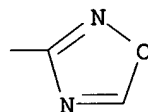
CM 1

CRN 622381-57-1  
 CMF C28 H26 N8 O2 S

PAGE 1-A

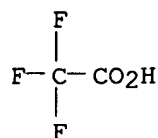


PAGE 1-B

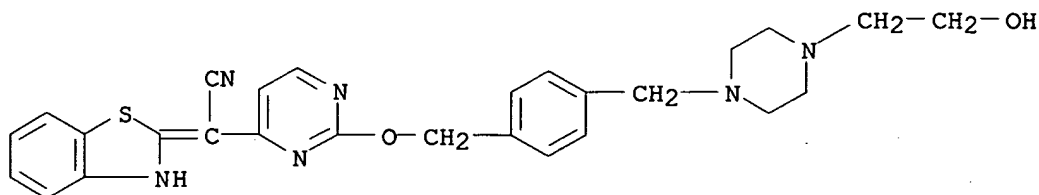


CM 2

CRN 76-05-1  
 CMF C2 H F3 O2



RN 622381-59-3 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[4-[[4-(2-hydroxyethyl)-1-piperazinyl]methyl]phenyl]methoxy]- (9CI) (CA INDEX NAME)

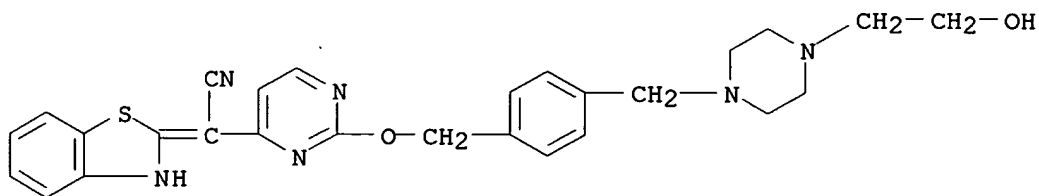
RN 622381-60-6 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[4-[[4-(2-hydroxyethyl)-1-piperazinyl]methyl]phenyl]methoxy]-, tris(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 622381-59-3

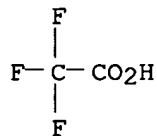
CMF C27 H28 N6 O2 S



CM 2

CRN 76-05-1

CMF C2 H F3 O2

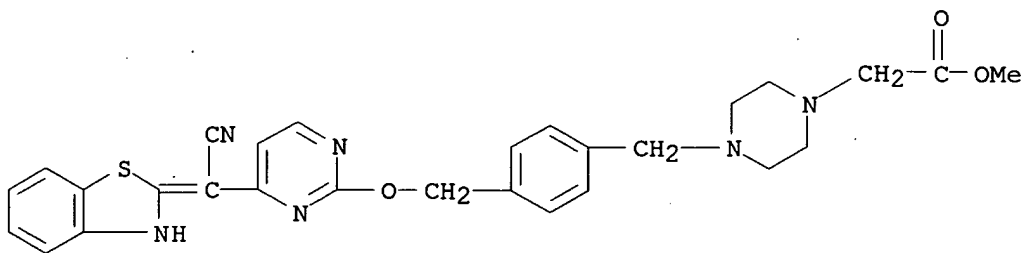


RN 622381-61-7 CAPLUS

CN 1-Piperazineacetic acid, 4-[[4-[[[4-(2(3H)-benzothiazolylidene)acetonitrile]methyl]phenyl]methoxy]-



2-pyrimidinyl]oxy)methyl]phenyl)methyl]-, methyl ester (9CI) (CA INDEX NAME)



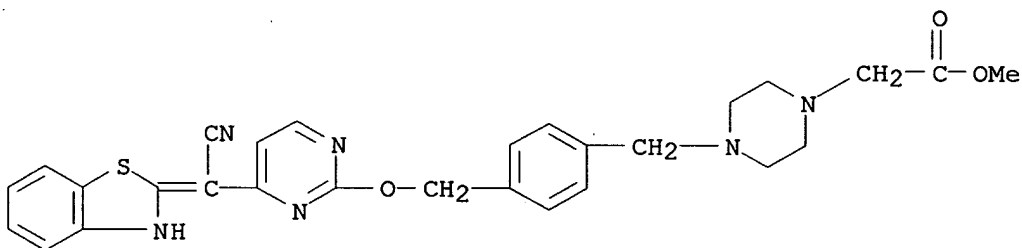
RN 622381-62-8 CAPLUS

CN 1-Piperazineacetic acid, 4-[[[4-[[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy)methyl]phenyl)methyl]-, methyl ester, tris(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 622381-61-7

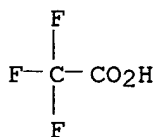
CMF C28 H28 N6 O3 S



CM 2

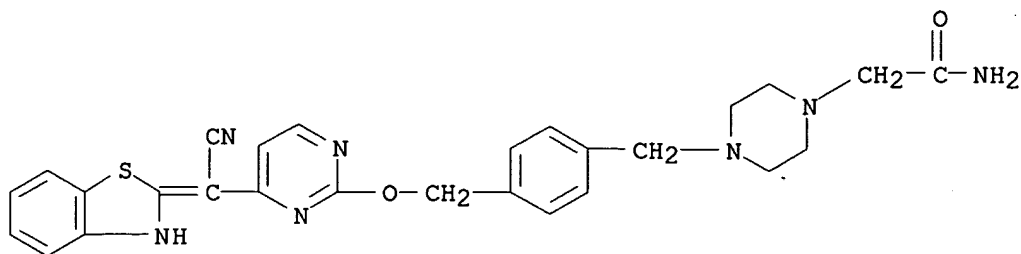
CRN 76-05-1

CMF C2 H F3 O2



RN 622381-63-9 CAPLUS

CN 1-Piperazineacetamide, 4-[[[4-[[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy)methyl]phenyl)methyl]- (9CI) (CA INDEX NAME)



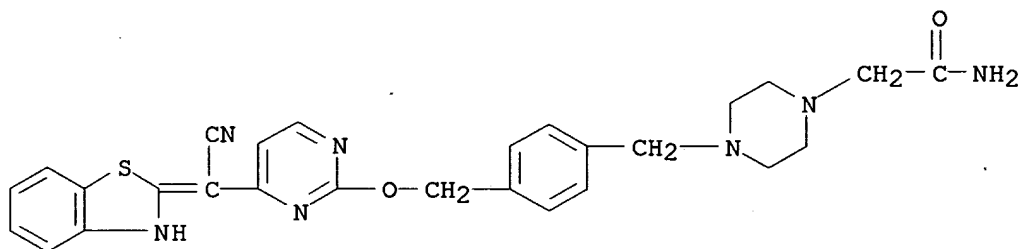
RN 622381-64-0 CAPLUS

CN 1-Piperazineacetamide, 4-[[[4-[[[4-(2(3H)-benzothiazolylidenecyanomethyl)-2-pyrimidinyl]oxy]methyl]phenyl]methyl]-, tris(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 622381-63-9

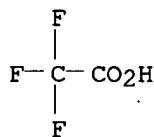
CMF C27 H27 N7 O2 S



CM 2

CRN 76-05-1

CMF C2 H F3 O2



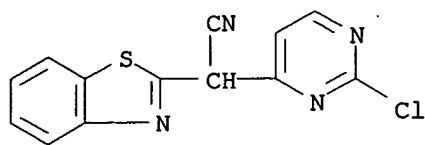
IT 345986-38-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of piperazine benzothiazoles as inhibitors of JNK kinases)

RN 345986-38-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, alpha-(2-chloro-4-pyrimidinyl)- (9CI) (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2003:454111 CAPLUS  
 DN 139:36533  
 TI Benzazole derivatives for the treatment of scleroderma  
 IN Gotteland, Jean-Pierre; Gaillard, Pascale; Chvatchko, Yolande  
 PA Applied Research Systems ARS Holding N.V., Neth.  
 SO PCT Int. Appl., 44 pp.  
 CODEN: PIXXD2

DT Patent  
 LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003047570	A1	20030612	WO 2002-EP13857	20021206
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2468826	AA	20030612	CA 2002-2468826	20021206
	AU 2002352227	A1	20030617	AU 2002-352227	20021206
	EP 1450792	A1	20040901	EP 2002-787919	20021206
	EP 1450792	B1	20060927		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
	JP 2005515994	T2	20050602	JP 2003-548825	20021206
	US 2005119277	A1	20050602	US 2003-496785	20021206
PRAI	EP 2001-727	A	20011207		
	WO 2002-EP13857	W	20021206		

OS MARPAT 139:36533

AB The present invention is related to the use of benzazole derivs. I [X = O, etc.; G = pyrimidinyl; R1 = H, alkoxy, etc.; R2 = H, alkyl, etc.] for the treatment and/or prevention of scleroderma and its therapeutic implications selected in the group consisting of systemic sclerosis, scleroderma-like disorders, liver cirrhosis, interstitial pulmonary fibrosis, Dupuytren's contracture, keloid and other scarring/wound healing abnormalities, postoperative adhesions, etc. The bioactivities of one compound of this invention were demonstrated. Formulations are given.

IT 541507-15-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzazole derivs. for treatment of scleroderma)

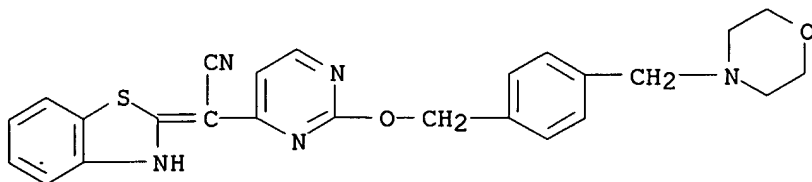
RN 541507-15-7 CAPLUS

CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolyldiene-2-[[4-(4-morpholinylmethyl)phenyl]methoxy]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 541507-14-6

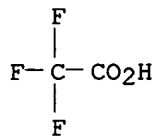
CMF C25 H23 N5 O2 S



CM 2

CRN 76-05-1

CMF C2 H F3 O2

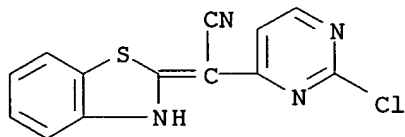


IT 541507-19-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of benzazole derivs. for treatment of scleroderma)

RN 541507-19-1 CAPLUS

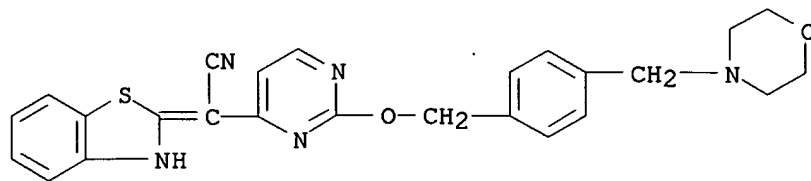
CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-chloro-  
(9CI) (CA INDEX NAME)

IT 541507-14-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(preparation of benzazole derivs. for treatment of scleroderma)

RN 541507-14-6 CAPLUS

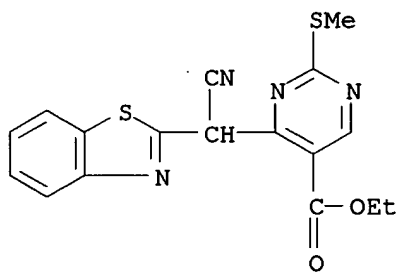
CN 4-Pyrimidineacetonitrile,  $\alpha$ -2(3H)-benzothiazolylidene-2-[[4-(4-morpholinylmethyl)phenyl]methoxy]- (9CI) (CA INDEX NAME)

RE.CNT 6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/511,438

L4 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2002:502303 CAPLUS  
 DN 138:24685  
 TI Reaction of 2-hetarylacetonitriles with ethyl 2-alkylsulfanyl-4-chloro-5-pyrimidinecarboxylates. Synthesis of new condensed pyrimidines  
 AU Blyumin, E. V.; Volovenko, Yu. M.; Neunhoeffer, Hans; Shishkina, S. V.; Zubatyuk, R. A.; Shishkin, Oleg V.  
 CS Chemical Department, Kiev Taras Shevchenko University, Kiev, 01033, Ukraine  
 SO Tetrahedron (2002), 58(28), 5733-5740  
 CODEN: TETRAB; ISSN: 0040-4020  
 PB Elsevier Science Ltd.  
 DT Journal  
 LA English  
 OS CASREACT 138:24685  
 AB Reactions of 2-hetarylacetonitriles  $R_1CH_2CN$  (I) ( $R_1$  = 2-pyridyl, 2-benzimidazolyl, 1-methyl-2-benzimidazolyl, 2-benzothiazolyl) with Et 2-alkylsulfanyl-4-chloro-5-pyrimidinecarboxylates II ( $R_2$  = Me,  $PhCH_2$ ) afforded a series of new condensed pyridopyrimidines, e.g. III. On the other hand, the analogous reaction of benzoxazole and 4-arylthiazole derived I, e.g. IV ( $R_3$  =  $Me_3C$ , 4- $ClC_6H_4$ , 4- $BrC_6H_4$ ), gave 4-[(2-hetaryl)-cyano-methyl]-2-alkylsulfanylpurimidine-5-carboxylates, e.g. V. Reactions of quinazoline derived I initially afforded stable intermediate similar to V which on heating with  $K_2CO_3$  formed the angular polycyclic compound VI. The influence of the basicity of heterocycles and of steric factors on the intramol. acylation reaction was studied.  
 IT 477879-90-6P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of (heteroaryl)pyrimidineacetonitriles and condensed pyridopyrimidines via condensation of heteroaryl acetonitriles with alkylthio(chloro)pyrimidinecarboxylates)  
 RN 477879-90-6 CAPLUS  
 CN 5-Pyrimidinecarboxylic acid, 4-(2-benzothiazolylcyanomethyl)-2-(methylthio)-, ethyl ester (9CI) (CA INDEX NAME)



RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2001:472001 CAPLUS  
 DN 135:61322  
 TI Preparation of benzazole derivatives as JNK modulators  
 IN Halazy, Serge; Church, Dennis; Camps, Montserrat; Gaillard, Pascale;  
 Gotteland, Jean-Pierre  
 PA Applied Research Systems Ars Holding N.V., Neth. Antilles  
 SO Eur. Pat. Appl., 31 pp.  
 CODEN: EPXXDW  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1110957	A1	20010627	EP 1999-811207	19991224
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	CA 2394809	AA	20010705	CA 2000-2394809	20001220
	WO 2001047920	A1	20010705	WO 2000-EP13006	20001220
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1240164	A1	20020918	EP 2000-991229	20001220
	EP 1240164	B1	20031112		
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	TR 200201509	T2	20020923	TR 2002-1509	20001220
	BR 2000016911	A	20021022	BR 2000-16911	20001220
	JP 2003519142	T2	20030617	JP 2001-549390	20001220
	EE 200200318	A	20031015	EE 2002-318	20001220
	AT 254123	E	20031115	AT 2000-991229	20001220
	PT 1240164	T	20040227	PT 2000-991229	20001220
	NZ 519423	A	20040430	NZ 2000-519423	20001220
	ES 2206351	T3	20040516	ES 2000-991229	20001220
	AU 780241	B2	20050310	AU 2001-31616	20001220
	ZA 2002004427	A	20040203	ZA 2002-4427	20020603
	BG 106830	A	20030228	BG 2002-106830	20020618
	NO 2002002997	A	20020621	NO 2002-2997	20020621
	US 2003162794	A1	20030828	US 2002-168718	20021021
	HK 1055730	A1	20060728	HK 2003-107978	20031105
PRAI	EP 1999-811207	A	19991224		
	WO 2000-EP13006	W	20001220		

OS MARPAT 135:61322

AB The title compds. [I; X = O, S, NR0; G = (un)substituted aryl, heteroaryl, 3-8-membered (un)saturated ring system containing at least one heteroatom selected

from N, O or S (said 3-8-membered ring system may be fused with (un)substituted aryl or heteroaryl system thus providing a bicyclic system); R1 = H, alkoxy, thioalkoxy, etc.; R2 = H, alkyl, alkenyl, etc.] which are efficient modulators of the JNK pathway, in particular efficient and selective inhibitors of JNK2 and/or 3, were prepared and formulated. E.g., a 2-step synthesis of I [X = S; R1, R2 = H; G = 2-[2-(1H-imidazol-4-



yl)ethylamino]-4-pyrimidinyl] which showed IC<sub>50</sub> of 70 nM and of 210 nM against JNK3 and JNK2, resp., was given.

IT 345986-38-1P 345986-40-5P 345986-44-9P

345986-46-1P 345986-48-3P 345986-50-7P

345986-64-3P 345986-65-4P 345986-66-5P

345986-67-6P 345986-69-8P 345986-70-1P

345986-72-3P 345986-73-4P 345986-75-6P

345986-76-7P 345986-78-9P 345986-79-0P

345986-81-4P 345986-82-5P 345986-84-7P

345986-85-8P 345986-86-9P 345986-87-0P

345986-88-1P 345986-89-2P 345986-91-6P

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345987-01-1P 345987-02-2P 345987-03-3P

345987-04-4P 345987-05-5P 345987-06-6P

345987-07-7P 345987-09-9P 345987-10-2P

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345987-14-6P 345987-15-7P 345987-16-8P

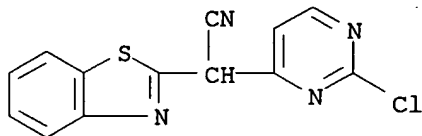
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzazole derivs. as JNK modulators)

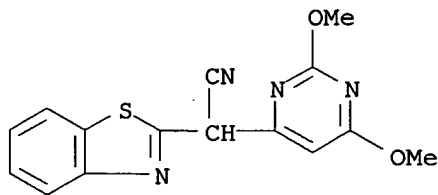
RN 345986-38-1 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -(2-chloro-4-pyrimidinyl)- (9CI) (CA INDEX NAME)



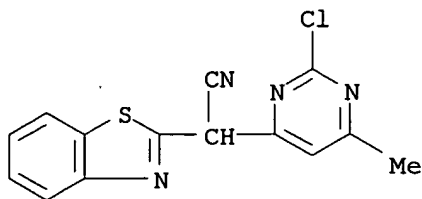
RN 345986-40-5 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -(2,6-dimethoxy-4-pyrimidinyl)- (9CI) (CA INDEX NAME)



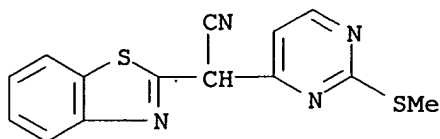
RN 345986-44-9 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -(2-chloro-6-methyl-4-pyrimidinyl)- (9CI) (CA INDEX NAME)



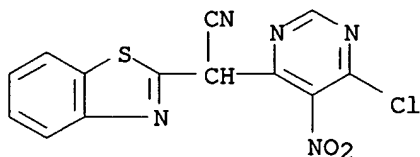
RN 345986-46-1 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(methylthio)-4-pyrimidinyl]- (9CI)  
(CA INDEX NAME)



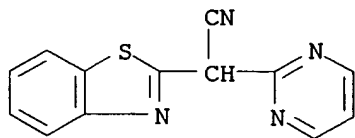
RN 345986-48-3 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -(6-chloro-5-nitro-4-pyrimidinyl)-  
(9CI) (CA INDEX NAME)



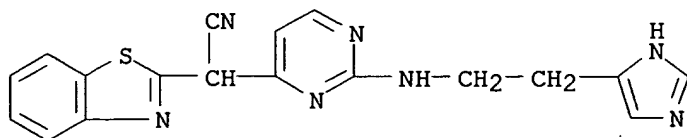
RN 345986-50-7 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -2-pyrimidinyl- (9CI) (CA INDEX NAME)



RN 345986-64-3 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(1H-imidazol-4-yl)ethyl]amino]-  
4-pyrimidinyl]- (9CI) (CA INDEX NAME)



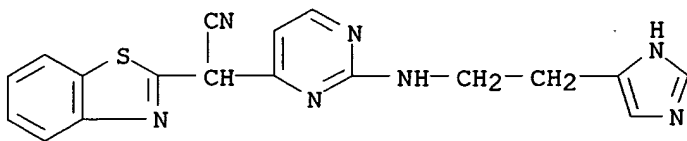
RN 345986-65-4 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(1H-imidazol-4-yl)ethyl]amino]-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1.

CRN 345986-64-3

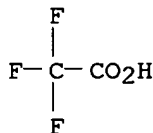
CMF C18 H15 N7 S



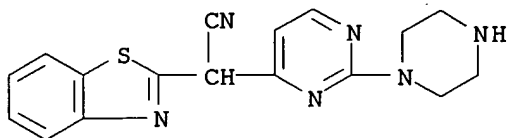
CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 345986-66-5 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(1-piperazinyl)-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

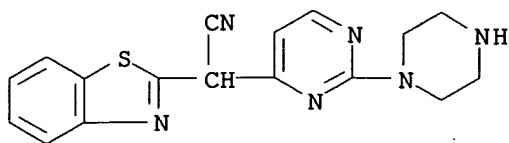
RN 345986-67-6 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(1-piperazinyl)-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345986-66-5

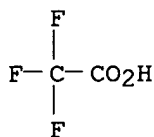
CMF C17 H16 N6 S



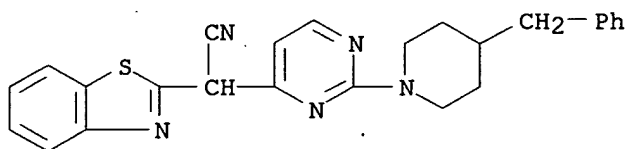
CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 345986-69-8 CAPLUS

CN 2-Benzothiazoleacetone nitrile,  $\alpha$ -[2-[4-(phenylmethyl)-1-piperidinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

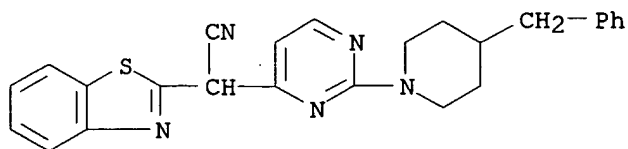
RN 345986-70-1 CAPLUS

CN 2-Benzothiazoleacetone nitrile,  $\alpha$ -[2-[4-(phenylmethyl)-1-piperidinyl]-4-pyrimidinyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345986-69-8

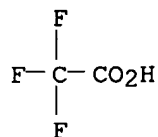
CMF C25 H23 N5 S



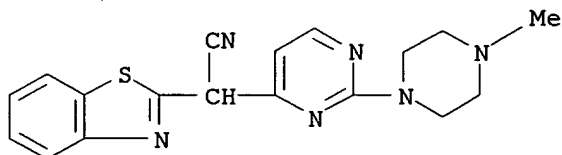
CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 345986-72-3 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(4-methyl-1-piperazinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

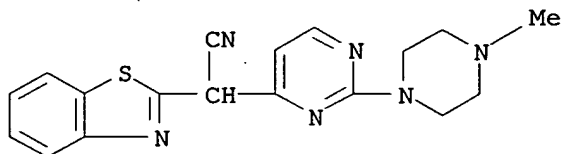
RN 345986-73-4 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(4-methyl-1-piperazinyl)-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345986-72-3

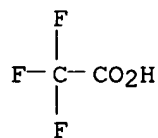
CMF C18 H18 N6 S



CM 2

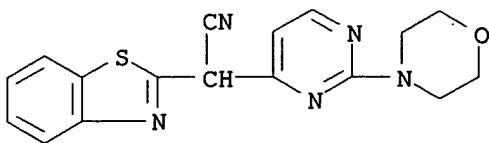
CRN 76-05-1

CMF C2 H F3 O2



RN 345986-75-6 CAPLUS

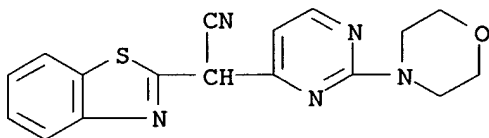
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(4-morpholinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 345986-76-7 CAPLUS  
 CN 2-Benzothiazoleacetone nitrile,  $\alpha$ -[2-(4-morpholinyl)-4-pyrimidinyl]-,  
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

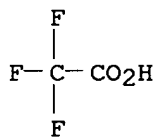
CM 1

CRN 345986-75-6  
 CMF C17 H15 N5 O S

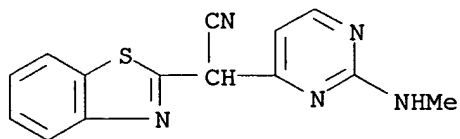


CM 2

CRN 76-05-1  
 CMF C2 H F3 O2



RN 345986-78-9 CAPLUS  
 CN 2-Benzothiazoleacetone nitrile,  $\alpha$ -[2-(methylamino)-4-pyrimidinyl]-,  
 (9CI) (CA INDEX NAME)

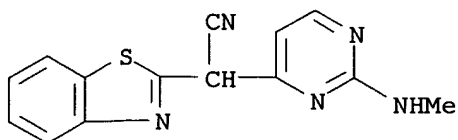


RN 345986-79-0 CAPLUS  
 CN 2-Benzothiazoleacetone nitrile,  $\alpha$ -[2-(methylamino)-4-pyrimidinyl]-,  
 mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345986-78-9

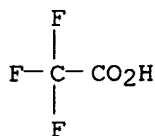
CMF C14 H11 N5 S



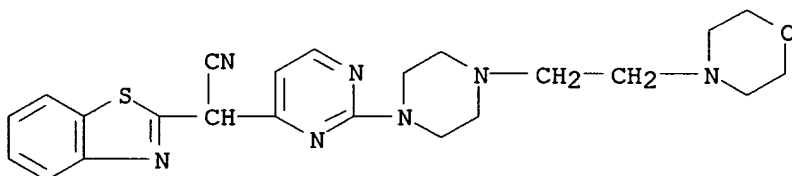
CM 2

CRN 76-05-1

CMF C2 H F3 O2



RN 345986-81-4 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[4-[2-(4-morpholinyl)ethyl]-1-piperazinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

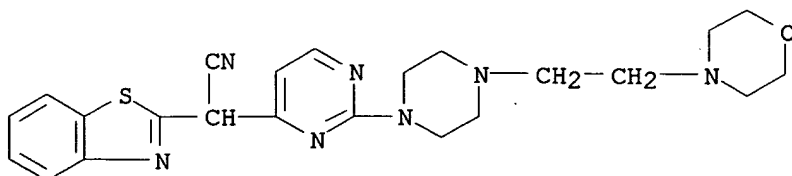
RN 345986-82-5 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[4-[2-(4-morpholinyl)ethyl]-1-piperazinyl]-4-pyrimidinyl]-, tris(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

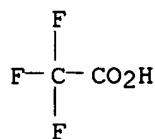
CRN 345986-81-4

CMF C23 H27 N7 O S

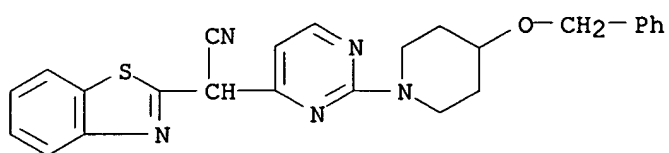


CM 2

CRN 76-05-1  
CMF C2 H F3 O2



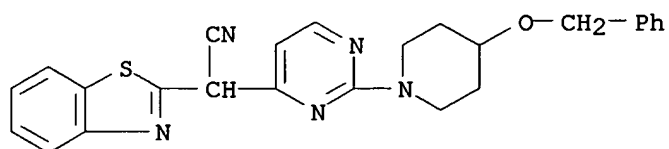
RN 345986-84-7 CAPLUS  
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[4-(phenylmethoxy)-1-piperidinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 345986-85-8 CAPLUS  
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[4-(phenylmethoxy)-1-piperidinyl]-4-pyrimidinyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

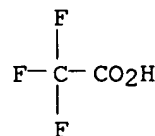
CM 1

CRN 345986-84-7  
CMF C25 H23 N5 O S



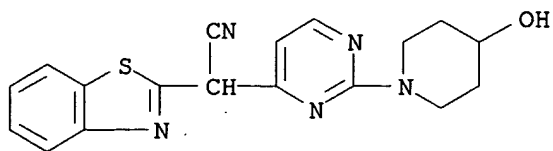
CM 2

CRN 76-05-1  
CMF C2 H F3 O2



RN 345986-86-9 CAPLUS  
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(4-hydroxy-1-piperidinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)





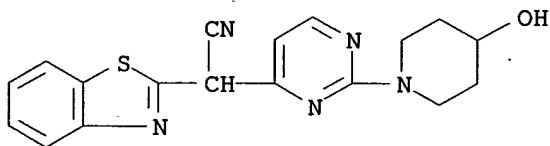
RN 345986-87-0 CAPLUS

CN 2-Benzothiazoleacetone nitrile,  $\alpha$ -[2-(4-hydroxy-1-piperidinyl)-4-pyrimidinyl]-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 345986-86-9

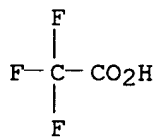
CMF C18 H17 N5 O S



CM 2

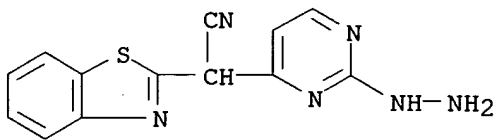
CRN 76-05-1

CMF C2 H F3 O2



RN 345986-88-1 CAPLUS

CN 2-Benzothiazoleacetone nitrile,  $\alpha$ -(2-hydrazino-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

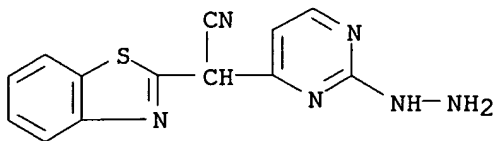


RN 345986-89-2 CAPLUS

CN 2-Benzothiazoleacetone nitrile,  $\alpha$ -(2-hydrazino-4-pyrimidinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

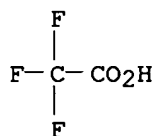
CM 1

CRN 345986-88-1  
CMF C13 H10 N6 S

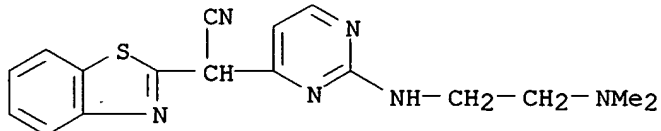


CM 2

CRN 76-05-1  
CMF C2 H F3 O2



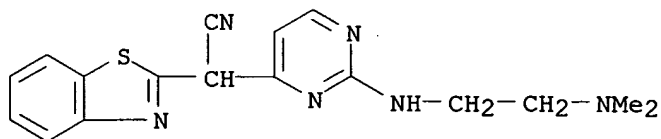
RN 345986-91-6 CAPLUS  
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(dimethylamino)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 345986-92-7 CAPLUS  
CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(dimethylamino)ethyl]amino]-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

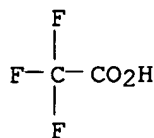
CRN 345986-91-6  
CMF C17 H18 N6 S



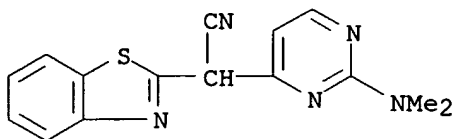
CM 2

CRN 76-05-1

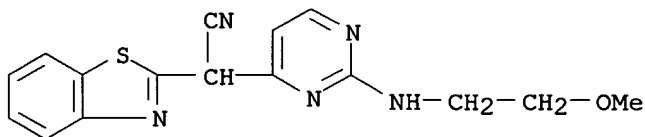
CMF C2 H F3 O2



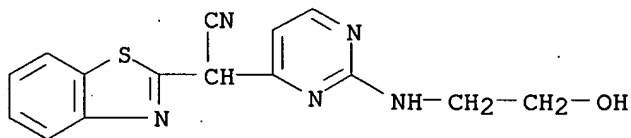
RN 345986-94-9 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(dimethylamino)-4-pyrimidinyl]-  
(9CI) (CA INDEX NAME)

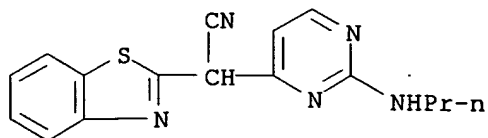
RN 345986-96-1 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[(2-methoxyethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

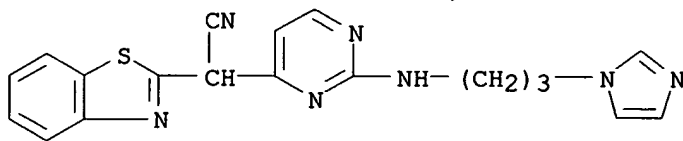
RN 345986-98-3 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[(2-hydroxyethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 345986-99-4 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(propylamino)-4-pyrimidinyl]-  
(9CI) (CA INDEX NAME)

RN 345987-00-0 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[3-(1H-imidazol-1-yl)propyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

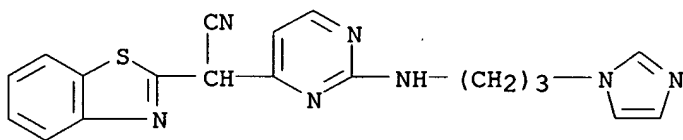
RN 345987-01-1 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[3-(1H-imidazol-1-yl)propyl]amino]-4-pyrimidinyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345987-00-0

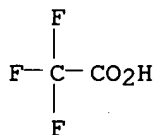
CMF C19 H17 N7 S



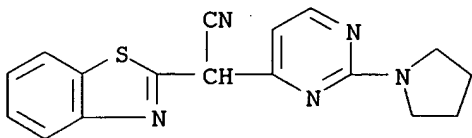
CM 2

CRN 76-05-1

CMF C2 H F3 O2



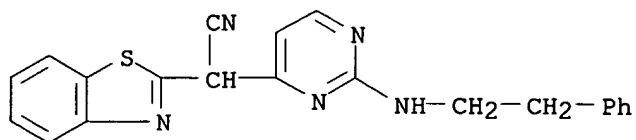
RN 345987-02-2 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-(1-pyrrolidinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

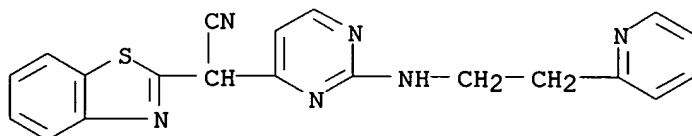
RN 345987-03-3 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[(2-phenylethyl)amino]-4-

pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 345987-04-4 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[(2-pyridinyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

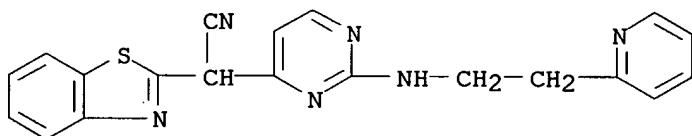
RN 345987-05-5 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[(2-pyridinyl)ethyl]amino]-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345987-04-4

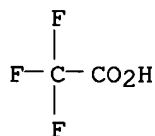
CMF C20 H16 N6 S



CM 2

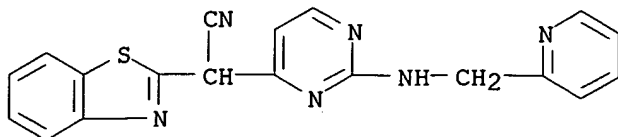
CRN 76-05-1

CMF C2 H F3 O2



RN 345987-06-6 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[(2-pyridinylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



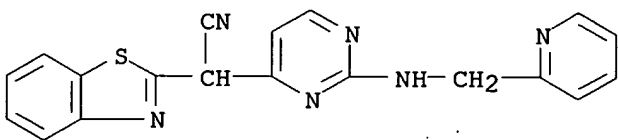
RN 345987-07-7 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[(2-pyridinylmethyl)amino]-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345987-06-6

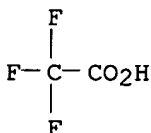
CMF C19 H14 N6 S



CM 2

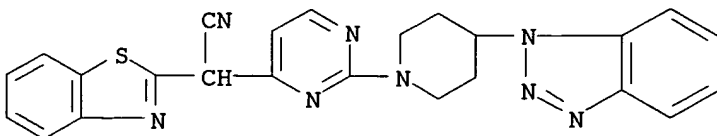
CRN 76-05-1

CMF C2 H F3 O2



RN 345987-09-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[4-(1H-benzotriazol-1-yl)-1-piperidinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



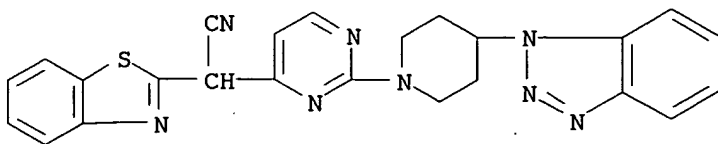
RN 345987-10-2 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[4-(1H-benzotriazol-1-yl)-1-piperidinyl]-4-pyrimidinyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345987-09-9

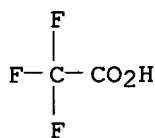
CMF C24 H20 N8 S



CM 2

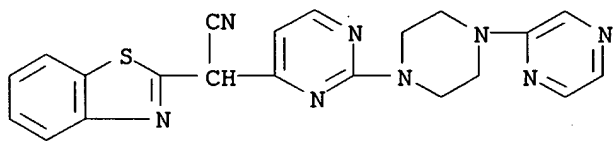
CRN 76-05-1

CMF C2 H F3 O2



RN 345987-11-3 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(4-pyrazinyl-1-piperazinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



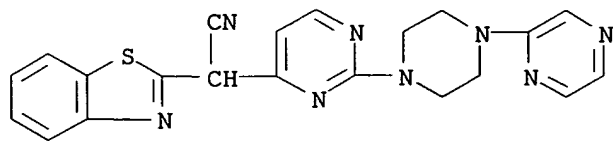
RN 345987-12-4 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-(4-pyrazinyl-1-piperazinyl)-4-pyrimidinyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345987-11-3

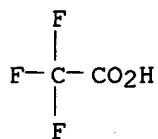
CMF C21 H18 N8 S



CM 2

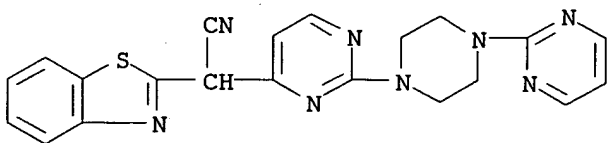
CRN 76-05-1

CMF C2 H F3 O2



RN 345987-13-5 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[4-(2-pyrimidinyl)-1-piperazinyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



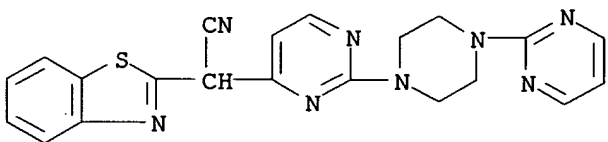
RN 345987-14-6 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[4-(2-pyrimidinyl)-1-piperazinyl]-4-pyrimidinyl]-, monò(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345987-13-5

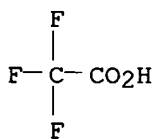
CMF C21 H18 N8 S



CM 2

CRN 76-05-1

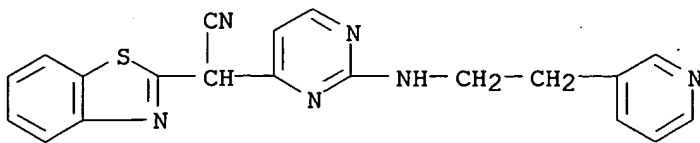
CMF C2 H F3 O2



RN 345987-15-7 CAPLUS

CN 2-Benzothiazoleacetonitrile,  $\alpha$ -[2-[[2-(3-pyridinyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)





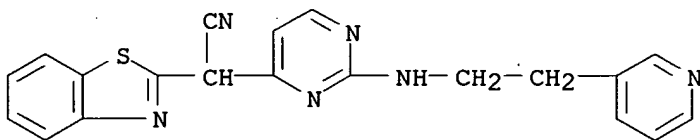
RN 345987-16-8 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[2-[[2-(3-pyridinyl)ethyl]amino]-4-pyrimidinyl]-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 345987-15-7

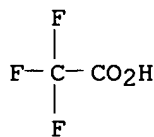
CMF C20 H16 N6 S



CM 2

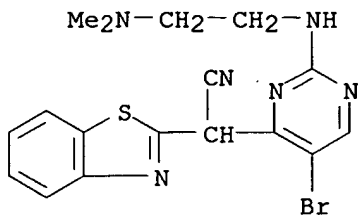
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CMF C2 H F3 O2



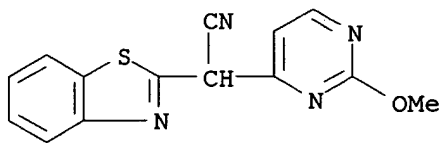
RN 345987-17-9 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-[5-bromo-2-[[2-(dimethylamino)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



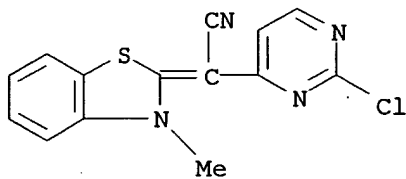
RN 345987-19-1 CAPLUS

CN 2-Benzothiazoleacetonitrile, α-(2-methoxy-4-pyrimidinyl)- (9CI) (CA INDEX NAME)



RN 345987-20-4 CAPLUS

CN 4-Pyrimidineacetonitrile, 2-chloro- $\alpha$ -(3-methyl-2(3H)-benzothiazolyldene)- (9CI) (CA INDEX NAME)



RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT